FIGURE 1

Amino acid sequence for full-length human wild type Cathepsin S [SEQ. ID No. 1]

Residues comprising the catalytic domain (~~115~~114-331) are underlined

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MKRLVCVLLV  CSSAVAQLHK  DPTLDHHWHL  WKKTYGKQYK  EKNEEAVRRL  IWEKNLKFVM   60
LHNLEHSMGM  HSYDLGMNHL  GDMTSEEVMS  LMSSLRVPSQ  WQRNITYKSN  PNRILPDSVD  120
WREKGCVTEV  KYQGSCGACW  AFSAVGALEA  QLKLKTGKLV  SLSAQNLVDC  STEKYGNKGC  180
NGGFMTTAFQ  YIIDNKGIDS  DASYPYKAMD  LKCQYDSKYR  AATCSKYTEL  PYGREDVLKE  240
AVANKGPVSV  GVDARHPSFF  LYRSGVYYEP  SCTQNVNHGV  LVVGYGDLNG  KEYWLVKNSW  300
GHNFGEEGYI  RMARNKGNHC  GIASFPSYPE  I                                  331
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Human cDNA sequence for Cathepsin S

[SEQ. ID No. 2]

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GCTTTCAGTG  CTGTGGGGGC  CCTGGAAGCA  CAGCTGAAGC  TGAAAACAGG  AAAGCTGGTG   480
TCTCTCAGTG  CCCAGAACCT  GGTGGATTGC  TCAACTGAAA  AATATGGAAA  CAAAGGCTGC   540
AATGGTGGCT  TCATGACAAC  GGCTTTCCAG  TACATCATTG  ATAACAAGGG  CATCGACTCA   600
GACGCTTCCT  ATCCCTACAA  AGCCATGGAT  CTGAAATGTC  AATATGACTC  AAAATATCGT   660
GCTGCCACAT  GTTCAAAGTA  CACTGAACTT  CCTTATGGCA  GAGAAGATGT  CCTGAAAGAA   720
GCTGTGGCCA  ATAAAGGCCC  AGTGTCTGTT  GGTGTAGATG  CGCGTCATCC  TTCTTTCTTC   780
CTCTACAGAA  GTGGTGTCTA  CTATGAACCA  TCCTGTACTC  AGAATGTGAA  TCATGGTGTA   840
CTTGTGGTTG  GCTATGGTGA  TCTTAATGGG  AAAGAATACT  GGCTTGTGAA  AAACAGCTGG   900
GGCCACAACT  TTGGTGAAGA  AGGATATATT  CGGATGGCAA  GAAATAAAGG  AAATCATTGT   960
GGGATTGCTA  GCTTTCCCTC  TTACCCAGAA  ATCTAG                             996
ATGAAACGGC  TGGTTTGTGT  GCTCTTGGTG  TGCTCCTCTG  CAGTGGCACA  GTTGCATAAA   60
GATCCTACCC  TGGATCACCA  CTGGCATCTC  TGGAAGAAAA  CCTATGGCAA  ACAATACAAG  120
GAAAAGAATG  AAGAAGCAGT  ACGACGTCTC  ATCTGGGAAA  AGAATCTAAA  GTTTGTGATG  180
CTTCACAACC  TGGAGCATTC  AATGGGAATG  CACTCATACG  ATCTGGGCAT  GAACCACCTG  240
GGAGACATGA  CCAGTGAAGA  AGTGATGTCT  TTGATGAGTT  CCCTGAGAGT  TCCCAGCCAG  300
TGGCAGAGAA  ATATCACATA  TAAGTCAAAC  CCTAATCGGA  TATTGCCTGA  TTCTGTGGAC  360
TGGAGAGAGA  AAGGGTGTGT  TACTGAAGTG  AAATATCAAG  GTTCTTGTGG  TGCTTGCTGG  420
GCTTTCAGTG  CTGTGGGGGC  CCTGGAAGCA  CAGCTGAAGC  TGAAAACAGG  AAAGCTGGTG  480
TCTCTCAGTG  CCCAGAACCT  GGTGGATTGC  TCAACTGAAA  AATATGGAAA  CAAAGGCTGC  540
AATGGTGGCT  TCATGACAAC  GGCTTTCCAG  TACATCATTG  ATAACAAGGG  CATCGACTCA  600
GACGCTTCCT  ATCCCTACAA  AGCCATGGAT  CTGAAATGTC  AATATGACTC  AAAATATCGT  660
GCTGCCACAT  GTTCAAAGTA  CACTGAACTT  CCTTATGGCA  GAGAAGATGT  CCTGAAAGAA  720
GCTGTGGCCA  ATAAAGGCCC  AGTGTCTGTT  GGTGTAGATG  CGCGTCATCC  TTCTTTCTTC  780
CTCTACAGAA  GTGGTGTCTA  CTATGAACCA  TCCTGTACTC  AGAATGTGAA  TCATGGTGTA  840
CTTGTGGTTG  GCTATGGTGA  TCTTAATGGG  AAAGAATACT  GGCTTGTGAA  AAACAGCTGG  900
GGCCACAACT  TTGGTGAAGA  AGGATATATT  CGGATGGCAA  GAAATAAAGG  AAATCATTGT  960
GGGATTGCTA  GCTTTCCCTC  TTACCCAGAA  ATCTAG                             996
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FIGURE 3

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	B	C	D	E	F	G	H	I	J
1	N	ILE	A	0——1	82.257	8.041	57.927	1.00	26.34
3	CA	ILE	A	0——1	82.504	8.282	59.377	1.00	25.81
5	CB	ILE	A	0——1	83.574	7.303	59.879	1.00	26.29
7	CG1	ILE	A	0——1	82.988	5.880	59.789	1.00	26.70
10	CD1	ILE	A	0——1	83.604	4.861	60.736	1.00	27.27
14	CG2	ILE	A	0——1	83.987	7.615	61.297	1.00	26.81
18	C	ILE	A	0——1	82.828	9.757	59.616	1.00	24.58
19	O	ILE	A	0——1	83.919	10.241	59.292	1.00	26.19
23	N	LEU	A	1——2	81.813	10.485	60.080	1.00	22.05
25	CA	LEU	A	1——2	81.954	11.891	60.442	1.00	20.00
27	CB	LEU	A	1——2	80.605	12.453	60.868	1.00	19.56
30	CG	LEU	A	1——2	79.501	12.355	59.825	1.00	20.01
32	CD1	LEU	A	1——2	78.222	12.934	60.367	1.00	21.60
36	CD2	LEU	A	1——2	79.905	13.043	58.524	1.00	19.14
40	C	LEU	A	1——2	82.941	12.101	61.574	1.00	18.72
41	O	LEU	A	1——2	83.100	11.254	62.440	1.00	18.37
42	N	PRO	A	2——3	83.604	13.243	61.569	1.00	17.60
43	CA	PRO	A	2——3	84.507	13.570	62.672	1.00	16.62
45	CB	PRO	A	2——3	85.045	14.949	62.305	1.00	17.14
48	CG	PRO	A	2——3	84.686	15.200	60.909	1.00	18.97
51	CD	PRO	A	2——3	83.548	14.300	60.560	1.00	17.68
54	C	PRO	A	2——3	83.723	13.654	63.967	1.00	15.96
55	O	PRO	A	2——3	82.565	14.052	63.934	1.00	15.78
56	N	ASP	A	3——4	84.338	13.302	65.087	1.00	15.34
58	CA	ASP	A	3——4	83.677	13.369	66.383	1.00	15.46
60	CB	ASP	A	3——4	84.503	12.677	67.469	1.00	16.27
63	CG	ASP	A	3——4	84.314	11.162	67.480	1.00	20.81
64	OD1	ASP	A	3——4	83.374	10.648	66.823	1.00	22.78
65	OD2	ASP	A	3——4	85.068	10.405	68.142	1.00	24.08
66	C	ASP	A	3——4	83.471	14.813	66.780	1.00	14.04
67	O	ASP	A	3——4	82.593	15.116	67.564	1.00	14.43
68	N	SER	A	4— 5	84.298	15.690	66.241	1.00	13.06
70	CA	SER	A	4— 5	84.165	17.107	66.525	1.00	13.20
72	CB	SER	A	4— 5	84.951	17.460	67.785	1.00	13.87
75	OG	SER	A	4— 5	86.328	17.434	67.527	1.00	15.53
77	C	SER	A	4— 5	84.589	17.965	65.344	1.00	12.32
78	O	SER	A	4— 5	85.435	17.579	64.535	1.00	12.78
79	N	VAL	A	5——A	6	83.964	19.130	65.229	1.00 11.07
81	CA	VAL	A	5——A	6	84.253	20.077	64.179	1.00 11.25
83	CB	VAL	A	5——A	6	83.156	20.009	63.094	1.00 11.71
85	CG1	VAL	A	5——A	6	83.239	21.160	62.144	1.00 12.21
89	CG2	VAL	A	5——A	6	83.218	18.674	62.379	1.00 12.06

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
93	C	VAL	A	5	A 6	84.244	21.476	64.765	1.00 10.82
94	O	VAL	A	5	A 6	83.468	21.747	65.667	1.00 10.70
95	N	ASP	A	6——7	85.092	22.360	64.250	1.00	11.43
97	CA	ASP	A	6——7	85.069	23.775	64.647	1.00	11.57
99	CB	ASP	A	6——7	85.927	24.038	65.878	1.00	11.62
102	CG	ASP	A	76	85.834	25.469	66.382	1.00	14.15
103	OD1	ASP	A	76	85.435	26.374	65.617	1.00	12.41
104	OD2	ASP	A	76	86.154	25.766	67.577	1.00	15.00
105	C	ASP	A	76	85.549	24.564	63.457	1.00	11.35
106	O	ASP	A	76	86.731	24.639	63.171	1.00	11.67
107	N	TRP	A	87	84.613	25.145	62.709	1.00	10.50
109	CA	TRP	A	87	84.938	25.857	61.503	1.00	10.47
111	CB	TRP	A	87	83.641	26.205	60.743	1.00	10.56
114	CG	TRP	A	87	83.120	25.010	59.975	1.00	10.28
115	CD1	TRP	A	87	82.073	24.218	60.294	1.00	10.49
117	NE1	TRP	A	87	81.956	23.200	59.372	1.00	9.78
119	CE2	TRP	A	87	82.932	23.340	58.429	1.00	10.67
120	CD2	TRP	A	87	83.696	24.459	58.788	1.00	11.28
121	CE3	TRP	A	87	84.759	24.830	57.964	1.00	13.13
123	CZ3	TRP	A	87	85.050	24.042	56.844	1.00	13.88
125	CH2	TRP	A	87	84.283	22.941	56.529	1.00	14.28
127	CZ2	TRP	A	87	83.215	22.571	57.301	1.00	14.21
129	C	TRP	A	87	85.809	27.075	61.704	1.00	10.85
130	O	TRP	A	87	86.371	27.596	60.745	1.00	11.66
131	N	ARG	A	98	85.899	27.550	62.949	1.00	11.57
133	CA	ARG	A	98	86.787	28.663	63.251	1.00	13.62
135	CB	ARG	A	98	86.643	29.102	64.687	1.00	13.51
138	CG	ARG	A	98	85.293	29.655	65.033	1.00	13.24
141	CD	ARG	A	98	85.175	30.056	66.498	1.00	13.68
144	NE	ARG	A	98	85.318	28.897	67.360	1.00	13.08
146	CZ	ARG	A	98	85.231	28.912	68.670	1.00	13.37
147	NH1	ARG	A	98	85.011	30.041	69.314	1.00	15.01
150	NH2	ARG	A	98	85.385	27.792	69.342	1.00	14.86
153	C	ARG	A	98	88.213	28.246	63.012	1.00	14.93
154	O	ARG	A	98	89.034	29.059	62.580	1.00	16.62
155	N	GLU	A	109	— 88.502	26.968	63.234	1.00	15.84
157	CA	GLU	A	109—	89.850	26.418	63.048	1.00	17.63
159	CB	GLU	A	109—	89.923	25.022	63.663	1.00	18.54
162	CG	GLU	A	109—	89.627	25.009	65.152	1.00	22.00
165	CD	GLU	A	109—	89.773	23.625	65.771	1.00	25.95
166	OE1	GLU	A	109—	89.739	22.619	65.021	1.00	28.16
167	OE2	GLU	A	109—	89.899	23.555	67.013	1.00	29.66
168	C	GLU	A	109—	90.271	26.371	61.576	1.00	17.42
169	O	GLU	A	109—	91.457	26.221	61.266	1.00	19.10
170	N	LYS	A	1110—	89.341	26.675	60.680	1.00	17.42
172	CA	LYS	A	1110—	89.519	26.539	59.243	1.00	17.25
174	CB	LYS	A	1110—	88.484	25.622	58.578	1.00	18.47
177	CG	LYS	A	1110—	88.472	24.203	59.091	1.00	21.87
180	CD	LYS	A	1110—	89.629	23.388	58.551	1.00	25.43
183	CE	LYS	A	1110—	90.038	22.289	59.530	1.00	27.42
186	NZ	LYS	A	1110—	91.186	21.494	59.043	1.00	29.82

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
190	C	LYS	A	1̶1̶1̶ 0	89.436	27.953	58.666	1.00	16.53
191	O	LYS	A	1̶1̶1̶0	89.478	28.143	57.461	1.00	16.98
192	N	GLY	A	12̶1̶1̶	89.295	28.949	59.537	1.00	15.66
194	CA	GLY	A	12̶1̶1̶	89.219	30.327	59.127	1.00	15.31
197	C	GLY	A	12̶1̶1̶	87.980	30.655	58.319	1.00	14.80
198	O	GLY	A	12̶1̶1̶	88.021	31.534	57.457	1.00	15.59
199	N	CYS	A	13̶1̶2̶	86.876	29.975	58.626	1.00	13.63
201	CA	CYS	A	13̶1̶2̶	85.658	30.135	57.830	1.00	12.55
203	CB	CYS	A	13̶1̶2̶	85.092	28.769	57.471	1.00	13.05
206	SG	CYS	A	13̶1̶2̶	86.053	27.854	56.234	1.00	15.75
207	C	CYS	A	13̶1̶2̶	84.592	30.927	58.568	1.00	12.31
208	O	CYS	A	13̶1̶2̶	83.460	31.041	58.086	1.00	11.54
209	N	VAL	A	13̶1̶3̶	84.954	31.478	59.721	1.00	10.44
211	CA	VAL	A	14̶1̶3̶	84.022	32.223	60.562	1.00	9.80
213	CB	VAL	A	14̶1̶3̶	83.761	31.473	61.864	1.00	9.69
215	CG1	VAL	A	14̶1̶3̶	82.724	32.200	62.693	1.00	10.02
219	CG2	VAL	A	14̶1̶3̶	83.311	30.024	61.590	1.00	11.13
223	C	VAL	A	14̶1̶3̶	84.535	33.629	60.871	1.00	9.61
224	O	VAL	A	14̶1̶3̶	85.649	33.799	61.374	1.00	11.18
225	N	THR	A	15̶1̶4̶	83.720	34.635	60.596	1.00	9.79
227	CA	THR	A	15̶1̶4̶	84.104	36.013	60.862	1.00	10.47
229	CB	THR	A	15̶1̶4̶	83.296	36.995	60.013	1.00	11.70
231	OG1	THR	A	15̶1̶4̶	81.906	36.874	60.346	1.00	12.19
233	CG2	THR	A	15̶1̶4̶	83.410	36.669	58.567	1.00	11.82
237	C	THR	A	15̶1̶4̶	83.929	36.357	62.324	1.00	11.20
238	O	THR	A	15̶1̶4̶	83.417	35.566	63.109	1.00	10.87
239	N	ALA	A	16̶1̶5̶	84.208	37.610	62.637	1.00	12.52
241	CA	ALA	A	16̶1̶5̶	84.188	38.078	64.011	1.00	12.09
243	CB	ALA	A	16̶1̶5̶	84.730	39.470	64.105	1.00	13.84
247	C	ALA	A	16̶1̶5̶	82.733	38.075	64.423	1.00	11.36
248	O	ALA	A	16̶1̶5̶	81.842	38.261	63.598	1.00	10.77
249	N	VAL	A	17̶1̶6̶	82.502	37.860	65.706	1.00	10.58
251	CA	VAL	A	17̶1̶6̶	81.177	37.921	66.268	1.00	10.11
253	CB	VAL	A	17̶1̶6̶	81.222	37.468	67.730	1.00	10.38
255	CG1	VAL	A	17̶1̶6̶	79.950	37.835	68.464	1.00	11.56
259	CG2	VAL	A	17̶1̶6̶	81.488	35.989	67.780	1.00	11.48
263	C	VAL	A	17̶1̶6̶	80.680	39.347	66.131	1.00	10.10
264	O	VAL	A	17̶1̶6̶	81.414	40.297	66.382	1.00	11.71
265	N	LYS	A	18̶1̶7̶	79.421	39.489	65.747	1.00	8.56
267	CA	LYS	A	18̶1̶7̶	78.792	40.761	65.539	1.00	9.55
269	CB	LYS	A	18̶1̶7̶	77.986	40.755	64.237	1.00	10.39
272	CG	LYS	A	18̶1̶7̶	78.766	40.394	62.990	1.00	10.71
275	CD	LYS	A	18̶1̶7̶	80.056	41.159	62.846	1.00	10.83
278	CE	LYS	A	18̶1̶7̶	80.725	40.971	61.474	1.00	12.15
281	NZ	LYS	A	18̶1̶7̶	81.129	39.568	61.143	1.00	12.51
285	C	LYS	A	18̶1̶7̶	77.842	41.082	66.692	1.00	9.43
286	O	LYS	A	18̶1̶7̶	77.494	40.224	67.484	1.00	9.72
287	N	TYR	A	19̶1̶8̶	77.424	42.346	66.754	1.00	10.36
289	CA	TYR	A	19̶1̶8̶	76.531	42.802	67.812	1.00	10.98
291	CB	TYR	A	19̶1̶8̶	77.250	43.834	68.694	1.00	11.20
294	CG	TYR	A	19̶1̶8̶	76.391	44.406	69.803	1.00	13.29

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
295	CD1	TYR	A	19~~18~~	75.859	45.676	69.695	1.00	16.23
297	CE1	TYR	A	19~~18~~	75.087	46.210	70.700	1.00	16.53
299	CZ	TYR	A	19~~18~~	74.821	45.481	71.814	1.00	19.68
301	CE2	TYR	A	19~~18~~	75.338	44.222	71.958	1.00	19.55
303	CD2	TYR	A	19~~18~~	76.124	43.683	70.945	1.00	16.47
305	C	TYR	A	19~~18~~	75.308	43.407	67.155	1.00	10.43
306	O	TYR	A	19~~18~~	75.395	44.464	66.506	1.00	11.82
307	N	GLN	A	20~~19~~	74.166	42.761	67.336	1.00	9.89
309	CA	GLN	A	20~~19~~	72.943	43.194	66.646	1.00	10.10
311	CB	GLN	A	20~~19~~	71.945	42.044	66.498	1.00	10.63
314	CG	GLN	A	20~~19~~	71.296	41.576	67.730	1.00	11.13
317	CD	GLN	A	20~~19~~	70.402	40.388	67.480	1.00	12.73
318	OE1	GLN	A	20~~19~~	70.875	39.244	67.381	1.00	12.94
319	NE2	GLN	A	20~~19~~	69.109	40.633	67.395	1.00	13.57
322	C	GLN	A	20~~19~~	72.280	44.376	67.310	1.00	11.11
323	O	GLN	A	20~~19~~	71.514	45.087	66.684	1.00	11.05
324	N	GLY	A	21~~20~~	72.605	44.624	68.563	1.00	11.36
326	CA	GLY	A	21~~20~~	71.950	45.707	69.287	1.00	12.15
329	C	GLY	A	21~~20~~	70.454	45.508	69.458	1.00	12.43
330	O	GLY	A	21~~20~~	69.955	44.383	69.498	1.00	12.85
331	N	SER	A	22~~21~~	69.688	46.606	69.468	1.00	13.09
333	CA	SER	A	22~~21~~	68.251	46.505	69.693	1.00	14.69
335	CB	SER	A	22~~21~~	67.754	47.740	70.441	1.00	14.53
338	OG	SER	A	22~~21~~	68.301	47.790	71.722	1.00	16.94
340	C	SER	A	22~~21~~	67.463	46.374	68.410	1.00	15.57
341	O	SER	A	22~~21~~	66.468	47.041	68.222	1.00	19.41
342	N	CYS	A	23~~22~~	67.963	45.589	67.480	1.00	15.80
344	CA	CYS	A	23~~22~~	67.330	45.386	66.197	1.00	15.60
346	CB	CYS	A	23~~22~~	68.238	45.961	65.104	1.00	15.66
349	SG	CYS	A	23~~22~~	67.819	45.633	63.382	1.00	17.03
350	C	CYS	A	24~~22~~	67.229	43.875	66.055	1.00	15.55
351	O	CYS	A	24~~22~~	68.251	43.209	66.183	1.00	17.33
352	N	GLY	A	24~~23~~	66.042	43.352	65.754	1.00	14.59
354	CA	GLY	A	24~~23~~	65.822	41.914	65.616	1.00	14.25
357	C	GLY	A	24~~23~~	66.312	41.400	64.277	1.00	13.64
358	O	GLY	A	24~~23~~	65.538	40.922	63.446	1.00	14.90
359	N	ALA	A	25~~24~~	67.609	41.536	64.056	1.00	12.48
361	CA	ALA	A	25~~24~~	68.219	41.150	62.789	1.00	12.26
363	CB	ALA	A	25~~24~~	69.141	42.264	62.322	1.00	12.36
367	C	ALA	A	25~~24~~	69.008	39.855	62.876	1.00	12.16
368	O	ALA	A	25~~24~~	69.858	39.580	62.038	1.00	11.56
369	N	CYS	A	26~~25~~	68.722	39.059	63.902	1.00	12.16
371	CA	CYS	A	26~~25~~	69.397	37.778	64.097	1.00	12.81
373	CB	CYS	A	26~~25~~	68.784	37.016	65.280	1.00	13.57
376	SG	CYS	A	26~~25~~	67.082	36.526	65.019	1.00	16.39
377	C	CYS	A	26~~25~~	69.366	36.937	62.821	1.00	10.60
378	O	CYS	A	26~~25~~	70.360	36.311	62.475	1.00	10.27
379	N	TRP	A	26~~26~~	68.236	36.942	62.141	1.00	9.62
381	CA	TRP	A	27~~26~~	68.044	36.178	60.924	1.00	9.30
383	CB	TRP	A	27~~26~~	66.628	36.374	60.377	1.00	9.21
386	CG	TRP	A	27~~26~~	66.280	37.802	60.086	1.00	9.70

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
387	CD1	TRP	A	~~27~~26	65.877	38.728	60.989	1.00	10.89
389	NE1	TRP	A	~~27~~26	65.640	39.931	60.374	1.00	9.72
391	CE2	TRP	A	~~27~~26	65.898	39.795	59.037	1.00	8.87
392	CD2	TRP	A	~~27~~26	66.315	38.457	58.832	1.00	8.08
393	CE3	TRP	A	~~27~~26	66.641	38.054	57.534	1.00	8.37
395	CZ3	TRP	A	~~27~~26	66.517	38.963	56.511	1.00	9.65
397	CH2	TRP	A	~~27~~26	66.129	40.292	56.759	1.00	9.26
399	CZ2	TRP	A	~~27~~26	65.813	40.717	58.012	1.00	10.67
401	C	TRP	A	~~27~~26	69.071	36.588	59.880	1.00	8.89
402	O	TRP	A	~~27~~26	69.601	35.740	59.140	1.00	8.97
403	N	ALA	A	~~28~~27	69.370	37.878	59.822	1.00	7.92
405	CA	ALA	A	~~28~~27	70.296	38.408	58.825	1.00	7.88
407	CB	ALA	A	~~28~~27	70.158	39.926	58.661	1.00	8.39
411	C	ALA	A	~~28~~27	71.715	38.023	59.179	1.00	8.24
412	O	ALA	A	~~28~~27	72.492	37.658	58.320	1.00	8.11
413	N	PHE	A	~~29~~28	72.067	38.103	60.457	1.00	8.15
415	CA	PHE	A	~~29~~28	73.381	37.681	60.872	1.00	7.56
417	CB	PHE	A	~~29~~28	73.631	38.067	62.339	1.00	8.09
420	CG	PHE	A	~~29~~28	73.899	39.523	62.518	1.00	8.52
421	CD1	PHE	A	~~29~~28	72.937	40.367	63.030	1.00	10.35
423	CE1	PHE	A	~~29~~28	73.180	41.738	63.140	1.00	11.21
425	CZ	PHE	A	~~29~~28	74.371	42.246	62.710	1.00	9.28
427	CE2	PHE	A	~~29~~28	75.306	41.431	62.157	1.00	10.01
429	CD2	PHE	A	~~29~~28	75.080	40.063	62.073	1.00	9.08
431	C	PHE	A	~~29~~28	73.593	36.210	60:653	1.00	7.36
432	O	PHE	A	~~29~~28	74.683	35.803	60.279	1.00	8.40
433	N	SER	A	~~32~~90 —	72.580	35.420	60.943	1.00	7.43
435	CA	SER	A	~~30~~29	72.669	33.984	60.763	1.00	7.87
437	CB	SER	A	~~30~~29	71.398	33.332	61.233	1.00	8.44
440	OG	SER	A	~~30~~29	71.436	31.948	60.941	1.00	8.69
442	C	SER	A	~~30~~29	72.912	33.665	59.298	1.00	7.91
443	O	SER	A	~~30~~29	73.800	32.889	58.957	1.00	8.20
444	N	ALA	A	~~31~~30	72.146	34.329	58.451	1.00	7.85
446	CA	ALA	A	~~31~~30	72.237	34.117	57.019	1.00	8.22
448	CB	ALA	A	~~31~~30	71.085	34.839	56.311	1.00	8.26
452	C	ALA	A	~~31~~30	73.589	34.575	56.463	1.00	8.69
453	O	ALA	A	~~32~~30	74.192	33.862	55.671	1.00	9.42
454	N	VAL	A	~~32~~31	74.076	35.733	56.872	1.00	8.72
456	CA	VAL	A	~~32~~31	75.353	36.156	56.337	1.00	9.28
458	CB	VAL	A	~~32~~31	75.675	37.659	56.586	1.00	10.50
460	CG1	VAL	A	~~32~~31	74.561	38.564	56.090	1.00	12.29
464	CG2	VAL	A	~~32~~31	75.949	37.927	57.999	1.00	11.66
468	C	VAL	A	~~32~~31	76.495	35.265	56.851	1.00	8.52
469	O	VAL	A	~~32~~31	77.453	35.022	56.130	1.00	8.68
470	N	GLY	A	~~33~~32	76.392	34.776	58.081	1.00	7.85
472	CA	GLY	A	~~33~~32	77.411	33.915	58.637	1.00	8.13
475	C	GLY	A	~~33~~32	77.594	32.644	57.842	1.00	7.86
476	O	GLY	A	~~33~~32	78.710	32.184	57.563	1.00	8.58
477	N	ALA	A	~~34~~33	76.459	32.052	57.473	1.00	8.26
479	CA	ALA	A	~~34~~33	76.472	30.838	56.676	1.00	7.48
481	CB	ALA	A	~~34~~33	75.083	30.353	56.481	1.00	8.24

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
485	C	ALA	A	34~~33~~	77.140	31.109	55.327	1.00	7.77
486	O	ALA	A	34~~33~~	77.918	30.301	54.834	1.00	8.24
487	N	LEU	A	35~~34~~	76.760	32.199	54.691	1.00	8.26
489	CA	LEU	A	35~~34~~	77.293	32.512	53.368	1.00	8.98
491	CB	LEU	A	35~~34~~	76.477	33.606	52.715	1.00	8.91
494	CG	LEU	A	35~~34~~	76.747	33.828	51.232	1.00	9.66
496	CD1	LEU	A	35~~34~~	76.569	32.534	50.402	1.00	11.47
500	CD2	LEU	A	35~~34~~	75.805	34.866	50.766	1.00	10.37
504	C	LEU	A	35~~34~~	78.775	32.854	53.399	1.00	9.66
505	O	LEU	A	35~~34~~	79.520	32.473	52.508	1.00	9.96
506	N	GLU	A	36~~35~~	79.196	33.541	54.449	1.00	10.00
508	CA	GLU	A	36~~35~~	80.610	33.894	54.609	1.00	9.89
510	CB	GLU	A	36~~35~~	80.819	34.665	55.932	1.00	11.60
513	CG	GLU	A	36~~35~~	80.206	36.067	55.965	1.00	12.79
516	CD	GLU	A	36~~35~~	79.998	36.642	57.364	1.00	13.45
517	OE1	GLU	A	36~~35~~	80.230	35.978	58.420	1.00	12.49
518	OE2	GLU	A	36~~35~~	79.582	37.809	57.412	1.00	12.98
519	C	GLU	A	36~~35~~	81.480	32.656	54.596	1.00	9.61
520	O	GLU	A	36~~35~~	82.558	32.670	54.017	1.00	9.71
521	N	ALA	A	37~~36~~	81.038	31.587	55.244	1.00	8.84
523	CA	ALA	A	37~~36~~	81.845	30.370	55.281	1.00	9.23
525	CB	ALA	A	37~~36~~	81.211	29.352	56.209	1.00	10.31
529	·C	ALA	A	37~~36~~	81.983	29.793	53.867	1.00	9.85
530	O	ALA	A	37~~36~~	83.065	29.383	53.428	1.00	9.44
531	N	GLN	A	38~~37~~	80.873	29.755	53.157	1.00	9.66
533	CA	GLN	A	38~~37~~	80.890	29.248	51.782	1.00	9.39
535	CB	GLN	A	38~~37~~	79.470	29.164	51.208	1.00	9.32
538	CG	GLN	A	38~~37~~	78.580	28.228	51.991	1.00	9.58
541	CD	GLN	A	38~~37~~	79.117	26.831	52.046	1.00	11.36
542	OE1	GLN	A	38~~37~~	79.515	26.281	51.017	1.00	12.35
543	NE2	GLN	A	38~~37~~	79.139	26.241	53.236	1.00	10.20
546	C	GLN	A	38~~37~~	81.771	30.106	50.894	1.00	9.59
547	O	GLN	A	38~~37~~	82.479	29.590	50.042	1.00	11.42
548	N	LEU	A	39~~38~~	81.775	31.419	51.119	1.00	9.82
550	CA	LEU	A	39~~38~~	82.615	32.322	50.339	1.00	9.67
552	CB	LEU	A	39~~38~~	82.276	33.763	50.674	1.00	10.76
555	CG	LEU	A	39~~38~~	83.111	34.826	49.966	1.00	11.15
557	CD1	LEU	A	39~~38~~	82.834	34.877	48.468	1.00	11.91
561	CD2	LEU	A	39~~38~~	82.855	36.147	50.574	1.00	11.50
565	C	LEU	A	39~~38~~	84.100	32.040	50.561	1.00	11.18
566	O	LEU	A	39~~38~~	84.885	31.977	49.625	1.00	11.71
567	N	LYS	A	40~~39~~	84.441	31.605	51.746	1.00	11.49
569	CA	LYS	A	40~~39~~	85.829	31.444	52.132	1.00	13.02
571	CB	LYS	A	40~~39~~	86.033	31.581	53.645	1.00	12.61
574	CG	LYS	A	40~~39~~	87.223	30.839	54.231	1.00	16.62
577	CD	LYS	A	40~~39~~	88.538	31.446	53.870	1.00	20.40
580	CE	LYS	A	40~~39~~	89.690	30.651	54.503	1.00	21.72
583	NZ	LYS	A	40~~39~~	89.233	29.337	55.032	1.00	28.53
587	C	LYS	A	40~~39~~	86.212	30.075	51.551	1.00	13.24
588	O	LYS	A	40~~39~~	87.289	29.917	50.943	1.00	13.01
589	N	LEU	A	41~~40~~	85.299	29.109	51.631	1.00	13.53

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
591	CA	LEU	A	4140	85.536	27.782	51.067	1.00	14.77
593	CB	LEU	A	4140	84.395	26.815	51.416	1.00	14.64
596	CG	LEU	A	4140	84.314	26.365	52.866	1.00	15.86
598	CD1	LEU	A	4140	82.988	25.629	53.172	1.00	16.87
602	CD2	LEU	A	4140	85.491	25.488	53.224	1.00	17.83
606	C	LEU	A	4140	85.735	27.863	49.545	1.00	15.17
607	O	LEU	A	4140	86.608	27.188	48.979	1.00	15.80
608	N	ALA	A	4241	85.046	28.787	48.903	1.00	15.49
610	CA	ALA	A	4241	85.019	28.884	47.458	1.00	16.60
612	CB	ALA	A	4241	83.687	29.459	46.969	1.00	17.33
616	C	ALA	A	4241	86.175	29.755	46.972	1.00	17.55
617	O	ALA	A	4241	86.818	29.432	45.963	1.00	18.46
618	N	THR	A	4342	86.453	30.857	47.662	1.00	16.62
620	CA	THR	A	4342	87.441	31.818	47.169	1.00	16.41
622	CB	THR	A	4342	86.828	33.206	47.115	1.00	16.85
624	OG1	THR	A	4342	86.616	33.713	48.449	1.00	15.15
626	CG2	THR	A	4342	85.483	33.160	46.458	1.00	17.28
630	C	THR	A	4342	88.706	31.932	47.972	1.00	16.79
631	O	THR	A	4342	89.679	32.553	47.515	1.00	16.90
632	N	GLY	A	4443	88.691	31.393	49.180	1.00	15.71
634	CA	GLY	A	4443	89.829	31.470	50.071	1.00	15.97
637	C	GLY	A	4443	89.844	32.748	50.891	1.00	15.78
638	O	GLY	A	4443	90.720	32.925	51.750	1.00	18.08
639	N	LYS	A	4544	88.888	33.641	50.638	1.00	14.70
641	CA	LYS	A	4544	88.828	34.921	51.327	1.00	14.35
643	CB	LYS	A	4544	88.524	36.037	50.348	1.00	14.89
646	CG	LYS	A	4544	89.588	36.220	49.276	1.00	16.99
649	CD	LYS	A	4544	89.353	37.471	48.497	1.00	19.33
652	CE	LYS	A	4544	90.447	37.641	47.446	1.00	22.13
655	NZ	LYS	A	4544	90.294	38.951	46.812	1.00	22.04
659	C	LYS	A	4544	87.745	34.931	52.384	1.00	13.26
660	O	LYS	A	4544	86.606	34.562	52.100	1.00	13.74
661	N	LEU	A	4645	88.102	35.362	53.587	1.00	11.64
663	CA	LEU	A	4645	87.154	35.533	54.676	1.00	11.56
665	CB	LEU	A	4645	87.771	35.156	56.019	1.00	11.55
668	CG	LEU	A	4645	86.766	35.211	57.164	1.00	13.05
670	CD1	LEU	A	4645	85.653	34.215	56.915	1.00	12.63
674	CD2	LEU	A	4645	87.433	34.929	58.475	1.00	14.82
678	C	LEU	A	4645	86.733	37.001	54.691	1.00	11.68
679	O	LEU	A	4645	87.519	37.888	55.018	1.00	12.55
680	N	VAL	A	4746	85.456	37.244	54.400	1.00	11.66
682	CA	VAL	A	4746	84.917	38.581	54.298	1.00	11.70
684	CB	VAL	A	4746	84.663	38.947	52.801	1.00	12.60
686	CG1	VAL	A	4746	84.118	40.336	52.678	1.00	14.24
690	CG2	VAL	A	4746	85.935	38.776	51.975	1.00	14.03
694	C	VAL	A	4746	83.574	38.659	55.015	1.00	11.12
695	O	VAL	A	4746	82.702	37.851	54.741	1.00	12.16
696	N	SER	A	4847	83.388	39.618	55.907	1.00	9.97
698	CA	SER	A	4847	82.093	39.805	56.538	1.00	9.81
700	CB	SER	A	4847	82.204	40.749	57.712	1.00	9.87
703	OG	SER	A	4847	82.806	40.089	58.826	1.00	11.68

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
705	C	SER	A	~~48~~47	81.147	40.402	55.517	1.00	9.76
706	O	SER	A	~~48~~47	81.479	41.378	54.837	1.00	10.20
707	N	LEU	A	~~49~~48	79.972	39.800	55.414	1.00	9.28
709	CA	LEU	A	~~49~~48	78.947	40.236	54.473	1.00	8.88
711	CB	LEU	A	~~49~~48	78.297	39.049	53.793	1.00	9.29
714	CG	LEU	A	~~49~~48	79.318	38.188	53.066	1.00	9.50
716	CD1	LEU	A	~~49~~48	78.677	36.909	52.544	1.00	9.17
720	CD2	LEU	A	~~49~~48	79.989	38.963	51.949	1.00	10.72
724	C	LEU	A	~~49~~48	77.931	41.100	55.204	1.00	9.30
725	O	LEU	A	~~49~~48	77.824	41.062	56.426	1.00	9.63
726	N	SER	A	~~50~~49	77.166	41.855	54.443	1.00	8.22
728	CA	SER	A	~~50~~49	76.319	42.877	55.009	1.00	8.41
730	CB	SER	A	~~50~~49	76.102	43.979	53.981	1.00	7.71
733	OG	SER	A	~~50~~49	75.262	44.969	54.515	1.00	8.95
735	C	SER	A	~~50~~49	74.948	42.411	55.513	1.00	8.25
736	O	SER	A	~~50~~49	74.035	42.196	54.732	1.00	7.24
737	N	ALA	A	~~51~~50	74.807	42.244	56.822	1.00	8.23
739	CA	ALA	A	~~51~~50	73.530	41.981	57.437	1.00	8.22
741	CB	ALA	A	~~51~~50	73.686	41.778	58.914	1.00	9.58
745	C	ALA	A	~~51~~50	72.585	43.155	57.170	1.00	8.52
746	O	ALA	A	~~51~~50	71.398	42.973	57.015	1.00	8.76
747	N	GLN	A	~~52~~51	73.122	44.364	57.108	1.00	8.59
749	CA	GLN	A	~~52~~51	72.297	45.543	56.887	1.00	8.33
751	CB	GLN	A	~~52~~51	73.113	46.841	57.004	1.00	8.51
754	CG	GLN	A	~~52~~51	72.217	48.056	57.014	1.00	9.63
757	CD	GLN	A	~~52~~51	71.387	48.139	58.270	1.00	11.05
758	OE1	GLN	A	~~52~~51	71.911	48.022	59.376	1.00	11.76
759	NE2	GLN	A	~~52~~51	70.064	48.317	58.105	1.00	11.59
762	C	GLN	A	~~52~~51	71.624	45.462	55.513	1.00	7.46
763	O	GLN	A	~~52~~51	70.463	45.835	55.360	1.00	9.03
764	N	ASN	A	~~53~~52	72.368	44.973	54.524	1.00	7.94
766	CA	ASN	A	~~53~~52	71.877	44.775	53.154	1.00	8.17
768	CB	ASN	A	~~53~~52	73.010	44.117	52.361	1.00	8.71
771	CG	ASN	A	~~53~~52	72.764	43.987	50.864	1.00	9.78
772	OD1	ASN	A	~~53~~52	73.715	43.784	50.139	1.00	9.29
773	ND2	ASN	A	~~53~~52	71.520	44.062	50.400	1.00	10.22
776	C	ASN	A	~~53~~52	70.630	43.903	53.228	1.00	8.45
777	O	ASN	A	~~53~~52	69.614	44.184	52.575	1.00	9.39
778	N	LEU	A	~~54~~53	70.671	42.836	54.004	1.00	8.18
780	CA	LEU	A	~~54~~53	69.500	41.992	54.159	1.00	8.18
782	CB	LEU	A	~~54~~53	69.880	40.772	54.949	1.00	7.76
785	CG	LEU	A	~~54~~53	70.186	39.458	54.243	1.00	13.79
787	CD1	LEU	A	~~54~~53	70.262	39.403	52.719	1.00	8.45
791	CD2	LEU	A	~~54~~53	71.181	38.560	54.955	1.00	10.18
795	C	LEU	A	~~54~~53	68.366	42.737	54.865	1.00	8.34
796	O	LEU	A	~~54~~53	67.212	42.739	54.420	1.00	8.16
797	N	VAL	A	~~55~~54	68.673	43.399	55.967	1.00	8.48
799	CA	VAL	A	~~55~~54	67.643	44.115	56.709	1.00	9.52
801	CB	VAL	A	~~55~~54	68.235	44.839	57.920	1.00	9.28
803	CG1	VAL	A	~~55~~54	67.256	45.856	58.503	1.00	10.40
807	CG2	VAL	A	~~55~~54	68.648	43.819	58.958	1.00	10.57

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
811	C	VAL	A	55~~54~~	66.863	45.098	55.848	1.00	10.23
812	O	VAL	A	~~54~~——55	65.645	45.216	55.955	1.00	10.25
813	N	ASP	A	56~~55~~	67.611	45.834	55.019	1.00	9.86
815	CA	ASP	A	56~~55~~	67.059	46.911	54.217	1.00	10.61
817	CB	ASP	A	56~~55~~	68.138	47.920	53.816	1.00	10.86
820	CG	ASP	A	56~~55~~	68.782	48.643	54.966	1.00	11.97
821	OD1	ASP	A	56~~55~~	68.248	48.677	56.097	1.00	11.58
822	OD2	ASP	A	56~~55~~	69.829	49.316	54.755	1.00	13.77
823	C	ASP	A	56~~55~~	66.464	46.460	52.904	1.00	11.01
824	O	ASP	A	56~~55~~	65.590	47.143	52.369	1.00	11.28
825	N	CYS	A	57~~56~~	66.967	45.356	52.369	1.00	10.95
827	CA	CYS	A	57~~56~~	66.615	44.945	51.016	1.00	11.42
829	CB	CYS	A	57~~56~~	67.872	44.800	50.159	1.00	12.43
832	SG	CYS	A	57~~56~~	68.897	46.285	50.192	1.00	13.92
833	C	CYS	A	57~~56~~	65.812	43.681	50.895	1.00	11.72
834	O	CYS	A	57~~56~~	65.031	43.551	49.946	1.00	12.21
835	N	SER	A	58~~57~~	66.016	42.725	51.787	1.00	10.84
837	CA	SER	A	58~~57~~	65.268	41.472	51.753	1.00	10.61
839	CB	SER	A	58~~57~~	66.126	40.323	52.295	1.00	10.76
842	OG	SER	A	58~~57~~	65.428	39.103	52.285	1.00	11.12
844	C	SER	A	58~~57~~	64.091	41.714	52.656	1.00	10.65
845	O	SER	A	58~~57~~	64.104	41.339	53.815	1.00	10.18
846	N	THR	A	59~~58~~	63.069	42.372	52.119	1.00	10.99
848	CA	THR	A	59~~58~~	61.995	42.873	52.964	1.00	11.26
850	CB	THR	A	59~~58~~	61.860	44.394	52.821	1.00	11.69
852	OG1	THR	A	59~~58~~	61.811	44.753	51.444	1.00	14.33
854	CG2	THR	A	59~~58~~	63.110	45.104	53.357	1.00	12.46
858	C	THR	A	59~~58~~	60.683	42.161	52.703	1.00	11.35
859	O	THR	A	59~~58~~	60.650	40.953	52.702	1.00	9.51
860	N	GLU	A	60~~59~~	59.609	42.903	52.512	1.00	12.57
862	CA	GLU	A	60~~59~~	58.291	42.289	52.443	1.00	13.36
864	CB	GLU	A	60~~59~~	57.237	43.375	52.248	1.00	15.43
867	CG	GLU	A	60~~59~~	57.314	44.112	50.949	1.00	19.60
870	CD	GLU	A	60~~59~~	58.226	45.341	50.986	1.00	24.88
871	OE1	GLU	A	60~~59~~	58.376	45.966	49.904	1.00	33.16
872	OE2	GLU	A	60~~59~~	58.785	45.678	52.075	1.00	22.39
873	C	GLU	A	60~~59~~	58.103	41.182	51.409	1.00	12.79
874	O	GLU	A	60~~59~~	57.394	40.200	51.668	1.00	12.73
875	N	LYS	A	61~~60~~	58.755	41.300	50.264	1.00	12.42
877	CA	LYS	A	61~~60~~	58.598	40.289	49.238	1.00	12.20
879	CB	LYS	A	61~~60~~	59.282	40.704	47.954	1.00	13.66
882	CG	LYS	A	61~~60~~	58.587	41.891	47.308	1.00	19.06
885	CD	LYS	A	61~~60~~	59.032	42.058	45.877	1.00	24.18
888	CE	LYS	A	61~~60~~	57.994	42.804	45.067	1.00	28.09
891	NZ	LYS	A	61~~60~~	56.687	42.062	45.085	1.00	31.37
895	C	LYS	A	61~~60~~	59.165	38.958	49.695	1.00	11.07
896	O	LYS	A	61~~60~~	58.833	37.916	49.146	1.00	11.28
897	N	TYR	A	62~~61~~	60.043	39.012	50.696	1.00	8.88
899	CA	TYR	A	62~~61~~	60.706	37.841	51.240	1.00	8.58
901	CB	TYR	A	62~~61~~	62.220	38.087	51.317	1.00	8.55
904	CG	TYR	A	62~~61~~	62.769	38.216	49.942	1.00	8.17

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
905	CD1	TYR	A	62~~61~~	62.915	39.453	49.335	1.00	8.94
907	CE1	TYR	A	62~~61~~	63.372	39.548	48.053	1.00	9.49
909	CZ	TYR	A	62~~61~~	63.682	38.421	47.354	1.00	10.13
910	OH	TYR	A	62~~61~~	64.131	38.536	46.068	1.00	12.74
912	CE2	TYR	A	62~~61~~	63.519	37.185	47.913	1.00	9.66
914	CD2	TYR	A	62~~61~~	63.083	37.091	49.219	1.00	8.09
916	C	TYR	A	62~~61~~	60.139	37.438	52.591	1.00	9.11
917	O	TYR	A	62~~61~~	60.641	36.532	53.255	1.00	9.78
918	N	GLY	A	63~~62~~	59.065	38.106	52.996	1.00	9.58
920	CA	GLY	A	63~~62~~	58.426	37.782	54.258	1.00	10.70
923	C	GLY	A	63~~62~~	59.202	38.249	55.485	1.00	10.96
924	O	GLY	A	63~~62~~	58.839	37.883	56.596	1.00	12.09
925	N	ASN	A	64~~63~~	60.260	39.030	55.287	1.00	10.88
927	CA	ASN	A	64~~63~~	61.064	39.585	56.390	1.00	10.67
929	CB	ASN	A	64~~63~~	62.533	39.520	56.039	1.00	10.44
932	CG	ASN	A	64~~63~~	62.948	38.144	55.666	1.00	9.70
933	OD1	ASN	A	64~~63~~	62.551	37.163	56.268	1.00	11.46
934	ND2	ASN	A	64~~63~~	63.803	38.089	54.658	1.00	10.82
937	C	ASN	A	64~~63~~	60.619	41.004	56.713	1.00	11.80
938	O	ASN	A	64~~63~~	60.106	41.699	55.842	1.00	14.10
939	N	ALA	A	65~~64~~	60.837	41.425	57.963	1.00	11.58
941	CA	ALA	A	65~~64~~	60.453	42.744	58.450	1.00	12.22
943	CB	ALA	A	65~~64~~	59.288	42.643	59.391	1.00	13.20
947	C	ALA	A	65~~64~~	61.620	43.459	59.121	1.00	12.25
948	O	ALA	A	65~~64~~	61.447	44.109	60.143	1.00	12.30
949	N	GLY	A	66~~65~~	62.809	43.296	58.560	1.00	11.56
951	CA	GLY	A	66~~65~~	63.974	44.032	58.999	1.00	11.65
954	C	GLY	A	66~~65~~	64.277	43.859	60.459	1.00	12.26
955	O	GLY	A	66~~65~~	64.526	42.755	60.911	1.00	11.35
956	N	CYS	A	67~~66~~	64.235	44.960	61.203	1.00	12.76
958	CA	CYS	A	67~~66~~	64.512	44.908	62.633	1.00	13.87
960	CB	CYS	A	67~~66~~	64.765	46.310	63.185	1.00	14.98
963	SG	CYS	A	67~~66~~	66.367	46.936	62.633	1.00	20.83
964	C	CYS	A	67~~66~~	63.432	44.209	63.444	1.00	13.60
965	O	CYS	A	67~~66~~	63.589	44.029	64.638	1.00	13.97
966	N	ASN	A	68~~67~~	62.344	43.804	62.795	1.00	12.40
968	CA	ASN	A	68~~67~~	61.276	43.111	63.478	1.00	13.63
970	CB	ASN	A	68~~67~~	59.954	43.843	63.288	1.00	13.48
973	CG	ASN	A	68~~67~~	59.831	45.020	64.227	1.00	16.37
974	OD1	ASN	A	68~~67~~	59.655	44.838	65.425	1.00	19.66
975	ND2	ASN	A	68~~67~~	59.992	46.216	63.702	1.00	17.62
978	C	ASN	A	68~~67~~	61.188	41.651	63.052	1.00	13.20
979	O	ASN	A	68~~67~~	60.159	41.002	63.211	1.00	15.60
980	N	GLY	A	69~~68~~	62.284	41.126	62.506	1.00	12.13
982	CA	GLY	A	69~~68~~	62.370	39.705	62.246	1.00	10.81
985	C	GLY	A	69~~68~~	62.347	39.303	60.795	1.00	10.90
986	O	GLY	A	69~~68~~	61.908	40.051	59.924	1.00	11.79
987	N	GLY	A	70~~69~~	62.832	38.102	60.546	1.00	9.81
989	CA	GLY	A	70~~69~~	62.887	37.573	59.207	1.00	9.19
992	C	GLY	A	70~~69~~	63.291	36.117	59.210	1.00	9.71
993	O	GLY	A	70~~69~~	63.359	35.487	60.251	1.00	9.76

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
994	N	PHE	A	71~~70~~	63.593	35.600	58.028	1.00	8.93
996	CA	PHE	A	71~~70~~	63.939	34.214	57.837	1.00	9.61
998	CB	PHE	A	71~~70~~	62.906	33.562	56.921	1.00	9.47
1001	CG	PHE	A	71~~70~~	61.503	33.587	57.458	1.00	12.32
1002	CD1	PHE	A	71~~70~~	60.577	34.511	57.007	1.00	15.23
1004	CE1	PHE	A	71~~70~~	59.270	34.515	57.508	1.00	16.98
1006	CZ	PHE	A	71~~70~~	58.903	33.601	58.461	1.00	17.37
1008	CE2	PHE	A	71~~70~~	59.810	32.696	58.918	1.00	18.52
1010	CD2	PHE	A	71~~70~~	61.110	32.675	58.405	1.00	16.82
1012	C	PHE	A	71~~70~~	65.279	34.080	57.169	1.00	9.78
1013	O	PHE	A	71~~70~~	65.573	34.842	56.269	1.00	9.49
1014	N	MET	A	72~~71~~	66.092	33.103	57.571	1.00	8.77
1016	CA	MET	A	72~~71~~	67.366	32.893	56.923	1.00	8.42
1018	CB	MET	A	72~~71~~	68.253	31.937	57.707	1.00	8.41
1021	CG	MET	A	72~~71~~	·68.778	32.526	59.001	1.00	8.98
1024	SD	MET	A	72~~71~~	67.633	32.408	60.355	1.00	10.95
1025	CE	MET	A	72~~71~~	67.802	30.753	60.771	1.00	11.40
1029	C	MET	A	72~~71~~	67.190	32.397	55.496	1.00	8.50
1030	O	MET	A	72~~71~~	67.876	32.845	54.605	1.00	9.24
1031	N	THR	A	73~~72~~	66.248	31.469	55.277	1.00	8.71
1033	CA	THR	A	73~~72~~	66.041	30.918	53.935	1.00	9.14
1035	CB	THR	A	73~~72~~	65.010	29.798	53.940	1.00	10.51
1037	OG1	THR	A	73~~72~~	63.814	30.236	54.589	1.00	12.31
1039	CG2	THR	A	73~~72~~	65.483	28.642	54.742	1.00	10.43
1043	C	THR	A	73~~72~~	65.607	31.981	52.959	1.00	8.69
1044	O	THR	A	73~~72~~	66.053	31.980	51.808	1.00	7.94
1045	N	THR	A	74~~73~~	64.710	32.874	53.366	1.00	7.74
1047	CA	THR	A	74~~73~~	64.255	33.872	52.395	1.00	8.53
1049	CB	THR	A	74~~73~~	62.935	34.503	52.747	1.00	9.08
1051	OG1	THR	A	74~~73~~	63.112	35.358	53.873	1.00	9.41
1053	CG2	THR	A	74~~73~~	61.937	33.471	53.152	1.00	10.41
1057	C	THR	A	74~~73~~	65.338	34.891	52.158	1.00	7.89
1058	O	THR	A	74~~73~~	65.416	35.472	51.081	1.00	9.88
1059	N	ALA	A	75~~74~~	66.188	35.113	53.159	1.00	8.72
1061	CA	ALA	A	75~~74~~	67.349	35.954	52.956	1.00	8.46
1063	CB	ALA	A	75~~74~~	68.126	36.104	54.247	1.00	8.87
1067	C	ALA	A	75~~74~~	68.254	35.352	51.869	1.00	8.67
1068	O	ALA	A	75~~74~~	68.756	36.062	50.997	1.00	7.71
1069	N	PHE	A	76~~75~~	68.483	34.046	51.929	1.00	8.62
1071	CA	PHE	A	76~~75~~	69.280	33.387	50.907	1.00	7.80
1073	CB	PHE	A	76~~75~~	69.467	31.880	51.165	1.00	7.93
1076	CG	PHE	A	76~~75~~	70.188	31.552	52.444	1.00	8.07
1077	CD1	PHE	A	76~~75~~	69.801	30.479	53.206	1.00	8.11
1079	CE1	PHE	A	76~~75~~	70.497	30.162	54.367	1.00	8.27
1081	CZ	PHE	A	76~~75~~	71.576	30.919	54.732	1.00	9.23
1083	CE2	PHE	A	76~~75~~	71.984	31.948	53.951	1.00	8.76
1085	CD2	PHE	A	76~~75~~	71.300	32.269	52.825	1.00	8.16
1087	C	PHE	A	76~~75~~	68.615	33.605	49.550	1.00	8.47
1088	O	PHE	A	76~~75~~	69.283	33.895	48.558	1.00	7.71
1089	N	GLN	A	77~~76~~	67.297	33.462	49.496	1.00	7.96
1091	CA	GLN	A	77~~76~~	66.626	33.605	48.206	1.00	8.60

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1093	CB	GLN	A	77~~76~~	65.163	33.204	48.298	1.00	8.91
1096	CG	GLN	A	77~~76~~	64.494	33.127	46.917	1.00	9.75
1099	CD	GLN	A	77~~76~~	65.106	32.047	46.007	1.00	9.93
1100	OE1	GLN	A	77~~76~~	65.336	30.917	46.434	1.00	12.13
1101	NE2	GLN	A	77~~76~~	65.348	32.402	44.733	1.00	11.34
1104	C	GLN	A	77~~76~~	66.796	35.002	47.677	1.00	8.48
1105	O	GLN	A	77~~76~~	66.975	35.186	46.484	1.00	8.43
1106	N	TYR	A	78~~77~~	66.727	36.001	48.547	1.00	8.18
1108	CA	TYR	A	78~~77~~	66.993	37.373	48.147	1.00	7.66
1110	CB	TYR	A	78~~77~~	66.808	38.371	49.315	1.00	7.86
1113	CG	TYR	A	78~~77~~	67.545	39.675	49.051	1.00	7.75
1114	CD1	TYR	A	78~~77~~	66.972	40.685	48.312	1.00	8.74
1116	CE1	TYR	A	78~~77~~	67.658	41.846	48.030	1.00	8.07
1118	CZ	TYR	A	78~~77~~	68.967	42.017	48.500	1.00	9.19
1119	OH	TYR	A	78~~77~~	69.658	43.178	48.214	1.00	10.00
1121	CE2	TYR	A	78~~77~~	69.557	41.014	49.242	1.00	8.23
1123	CD2	TYR	A	78~~77~~	68.861	39.851	49.488	1.00	8.01
1125	C	TYR	A	78~~77~~	68.383	37.497	47.519	1.00	8.03
1126	O	TYR	A	78~~77~~	68.564	38.088	46.467	1.00	8.18
1127	N	ILE	A	79~~78~~	69.385	36.911	48.144	1.00	7.87
1129	CA	ILE	A	79~~78~~	70.718	37.024	47.593	1.00	8.22
1131	CB	ILE	A	79~~78~~	71.743	36.393	48.551	1.00	8.27
1133	CG1	ILE	A	79~~78~~	71.696	37.098	49.889	1.00	8.93
1136	CD1	ILE	A	79~~78~~	72.532	36.457	50.938	1.00	9.31
1140	CG2	ILE	A	79~~78~~	73.143	36.514	47.986	1.00	8.27
1144	C	ILE	A	79~~78~~	70.788	36.384	46.205	1.00	8.54
1145	O	ILE	A	79~~78~~	71.428	36.933	45.286	1.00	9.65
1146	N	ILE	A	80~~79~~	70.097	35.266	46.042	1.00	8.96
1148	CA	ILE	A	80~~79~~	70.020	34.598	44.745	1.00	9.08
1150	CB	ILE	A	80~~79~~	69.271	33.268	44.851	1.00	9.18
1152	CG1	ILE	A	80~~79~~	70.065	32.285	45.717	1.00	9.39
1155	CD1	ILE	A	80~~79~~	69.265	31.099	46.122	1.00	11.40
1159	CG2	ILE	A	80~~79~~	68.998	32.713	43.470	1.00	11.43
1163	C	ILE	A	80~~79~~	69.346	35.509	43.744	1.00	9.68
1164	O	ILE	A	80~~79~~	69.898	35.795	42.669	1.00	10.88
1165	N	ASP	A	81~~80~~	68.159	35.973	44.087	1.00	10.14
1167	CA	ASP	A	81~~80~~	67.378	36.837	43.194	1.00	10.72
1169	CB	ASP	A	81~~80~~	66.058	37.201	43.848	1.00	11.65
1172	CG	ASP	A	81~~80~~	65.145	36.010	44.013	1.00	12.53
1173	OD1	ASP	A	81~~80~~	64.158	36.131	44.773	1.00	14.38
1174	OD2	ASP	A	81~~80~~	65.334	34.930	43.424	1.00	13.77
1175	C	ASP	A	81~~80~~	68.095	38.117	42.847	1.00	11.90
1176	O	ASP	A	81~~80~~	68.035	38.590	41.706	1.00	12.57
1177	N	ASN	A	82~~81~~	68.783	38.678	43.831	1.00	10.91
1179	CA	ASN	A	82~~81~~	69.470	39.966	43.692	1.00	11.60
1181	CB	ASN	A	82~~81~~	69.710	40.570	45.085	1.00	11.41
1184	CG	ASN	A	82~~81~~	70.127	42.002	45.031	1.00	12.60
1185	OD1	ASN	A	82~~81~~	69.430	42.837	44.477	1.00	12.65
1186	ND2	ASN	A	82~~81~~	71.277	42.309	45.620	1.00	11.59
1189	C	ASN	A	82~~81~~	70.805	39.855	42.970	1.00	11.62
1190	O	ASN	A	82~~81~~	71.409	40.875	42.613	1.00	12.76

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1191	N	LYS	A	8382	71.269	38.628	42.833	1.00	11.17
1193	CA	LYS	A	8382	72.534	38.317	42.179	1.00	11.77
1195	CB	LYS	A	8382	72.534	38.799	40.723	1.00	13.02
1198	CG	LYS	A	8382	71.424	38.104	39.923	1.00	16.14
1201	CD	LYS	A	8382	71.668	38.199	.38.438	1.00	21.01
1204	CE	LYS	A	8382	70.429	37.943	37.594	1.00	24.55
1207	NZ	LYS	A	8382	69.794	36.626	37.843	1.00	27.58
1211	C	LYS	A	8382	73.701	38.860	42.986	1.00	11.66
1212	O	LYS	A	8382	74.748	39.187	42.441	1.00	12.84
1213	N	GLY	A	8483	73.517	38.947	44.307	1.00	10.77
1215	CA	GLY	A	8483	74.605	39.370	45.155	1.00	10.74
1218	C	GLY	A	8483	74.222	39.972	46.482	1.00	10.21
1219	O	GLY	A	8483	73.079	40.320	46.761	1.00	9.37
1220	N	ILE	A	8584	75.239	40.121	47.324	1.00	8.79
1222	CA	ILE	A	8584	75.114	40.813	48.598	1.00	8.78
1224	CB	ILE	A	8584	74.882	39.805	49.758	1.00	8.92
1226	CG1	ILE	A	8584	74.678	40.543	51.074	1.00	8.01
1229	CD1	ILE	A	8584	74.298	39.603	52.203	1.00	9.78
1233	CG2	ILE	A	8584	76.016	38.796	49.885	1.00	8.34
1237	C	ILE	A	8584	76.402	41.604	48.786	1.00	8.57
1238	O	ILE	A	8584	77.471	41.130	48.424	1.00	9.25
1239	N	ASP	A	8685	76.290	42.792	49.348	1.00	8.93
1241	CA	ASP	A	8685	77.439	43.665	49.582	1.00	8.56
1243	CB	ASP	A	8685	76.967	45.086	49.777	1.00	9.03
1246	CG	ASP	A	8685	76.495	45.712	48.507	1.00	8.05
1247	OD1	ASP	A	8685	76.974	45.278	47.420	1.00	10.46
1248	OD2	ASP	A	8685	75.731	46.685	48.534	1.00	9.08
1249	C	ASP	A	8685	78.240	43.210	50.803	1.00	8.72
1250	O	ASP	A	8685	77.765	42.468	51.658	1.00	8.71
1251	N	SER	A	8786	79.469	43.661	50.873	1.00	9.41
1253	CA	SER	A	8786	80.273	43.400	52.056	1.00	9.29
1255	CB	SER	A	8786	81.734	43.744	51.771	1.00	9.72
1258	OG	SER	A	8786	81.871	45.137	51.637	1.00	10.12
1260	C	SER	A	8786	79.774	44.258	53.207	1.00	9.23
1261	O	SER	A	8786	79.166	45.290	53.030	1.00	8.87
1262	N	ASP	A	8887	80.058	43.819	54.423	1.00	9.52
1264	CA	ASP	A	8887	79.731	44.578	55.627	1.00	11.12
1266	CB	ASP	A	8887	80.115	43.730	56.838	1.00	11.26
1269	CG	ASP	A	8887	79.774	44.375	58.137	1.00	15.89
1270	OD1	ASP	A	8887	78.598	44.691	58.384	1.00	17.31
1271	OD2	ASP	A	8887	80.637	44.525	59.019	1.00	22.11
1272	C	ASP	A	8887	80.471	45.943	55.623	1.00	10.71
1273	O	ASP	A	8887	79.909	46.990	55.966	1.00	11.43
1274	N	ALA	A	8988	81.727	45.926	55.202	1.00	11.74
1276	CA	ALA	A	8988	82.512	47.173	55.121	1.00	11.97
1278	CB	ALA	A	8988	83.919	46.899	54.601	1.00	12.13
1282	C	ALA	A	8988	81.854	48.254	54.257	1.00	12.39
1284	N	SER	A	9089	81.246	47.770	53.174	1.00	11.37
1286	CA	SER	A	9089	80.644	48.666	52.207	1.00	12.12
1288	CB	SER	A	9089	80.601	48.009	50.829	1.00	11.86
1291	OG	SER	A	9089	79.623	46.974	50.742	1.00	14.44

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1293	C	SER	A	90~~89~~	79.250	49.099	52.585	1.00	12.03
1294	O	SER	A	90~~89~~	78.796	50.165	52.176	1.00	13.24
1295	N	TYR	A	91~~90~~	78.578	48.267	53.364	1.00	10.91
1297	CA	TYR	A	91~~90~~	77.171	48.462	53.699	1.00	10.77
1299	CB	TYR	A	91~~90~~	76.323	47.538	52.828	1.00	10.86
1302	CG	TYR	A	91~~90~~	74.857	47.900	52.704	1.00	9.36
1303	CD1	TYR	A	91~~90~~	74.209	48.625	53.678	1.00	10.28
1305	CE1	TYR	A	91~~90~~	72.896	48.949	53.575	1.00	9.06
1307	CZ	TYR	A	91~~90~~	72.169	48.538	52.476	1.00	11.94
1308	OH	TYR	A	91~~90~~	70.842	48.876	52.359	1.00	12.23
1311	CD2	TYR	A	91~~90~~	74.114	47.440	51.635	1.00	12.15
1312	C	TYR	A	91~~90~~	77.060	48.096	55.172	1.00	11.20
1313	O	TYR	A	91~~90~~	76.670	47.003	55.547	1.00	10.53
1314	N	PRO	A	92~~91~~	77.503	49.019	56.018	1.00	12.04
1315	CA	PRO	A	92~~91~~	77.639	48.729	57.447	1.00	12.68
1317	CB	PRO	A	92~~91~~	78.431	49.915	57.957	1.00	13.19
1320	CG	PRO	A	92~~91~~	78.872	50.585	56.760	1.00	15.61
1323	CD	PRO	A	92~~91~~	77.917	50.399	55.701	1.00	13.69
1326	C	PRO	A	92~~91~~	76.356	48.619	58.203	1.00	11.86
1327	O	PRO	A	92~~91~~	75.332	49.143	57.810	1.00	11.43
1328	N	TYR	A	93~~92~~	76.446	47.942	59.331	1.00	11.87
1330	CA	TYR	A	93~~92~~	75.271	47.655	60.131	1.00	11.07
1332	CB	TYR	A	93~~92~~	75.540	46.400	60.941	1.00	10.94
1335	CG	TYR	A	93~~92~~	74.367	45.954	61.770	1.00	10.33
1336	CD1	TYR	A	93~~92~~	73.225	45.444	61.177	1.00	9.36
1338	CE1	TYR	A	93~~92~~	72.151	45.042	61.947	1.00	9.94
1340	CZ	TYR	A	93~~92~~	72.215	45.176	63.308	1.00	10.19
1341	OH	TYR	A	93~~92~~	71.148	44.778	64.060	1.00	11.44
1343	CE2	TYR	A	93~~92~~	73.333	45.693	63.913	1.00	9.57
1345	CD2	TYR	A	93~~92~~	74.383	46.093	63.140	1.00	10.07
1347	C	TYR	A	93~~92~~	74.943	48.808	61.050	1.00	12.05
1348	O	TYR	A	93~~92~~	75.817	49.280	61.783	1.00	13.21
1349	N	LYS	A	94~~93~~	73.691	49.245	61.011	1.00	12.38
1351	CA	LYS	A	94~~93~~	73.250	50.387	61.790	1.00	13.76
1353	CB	LYS	A	94~~93~~	72.690	51.432	60.845	1.00	15.11
1356	CG	LYS	A	94~~93~~	73.668	51.887	59.776	1.00	17.85
1359	CD	LYS	A	94~~93~~	74.784	52.654	60.385	1.00	23.31
1362	CE	LYS	A	94~~93~~	75.753	53.161	59.342	1.00	26.53
1365	NZ	LYS	A	94~~93~~	76.764	54.033	59.984	1.00	29.62
1369	C	LYS	A	94~~93~~	72.184	50.052	62.814	1.00	13.22
1370	O	LYS	A	94~~93~~	71.735	50.925	63.556	1.00	13.40
1371	N	ALA	A	95~~94~~	71.763	48.798	62.851	1.00	12.76
1373	CA	ALA	A	95~~94~~	70.758	48.332	63.805	1.00	12.89
1375	CB	ALA	A	95~~94~~	71.297	48.339	65.242	1.00	12.52
1379	C	ALA	A	95~~94~~	69.456	49.125	63.699	1.00	13.54
1380	O	ALA	A	95~~94~~	68.818	49.449	64.715	1.00	13.99
1381	N	MET	A	96~~95~~	69.091	49.453	62.472	1.00	13.83
1383	CA	MET	A	96~~95~~	67.842	50.135	62.181	1.00	14.33
1385	CB	MET	A	96~~95~~	68.016	51.646	62.301	1.00	16.16
1389	SD	MET	A	96~~95~~	69.058	54.164	62.344	1.00	38.83
1390	CE	MET	A	96~~95~~	68.589	54.315	64.043	1.00	39.15

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1391	C	MET	A	9695	67.398	49.801	60.775	1.00	14.77
1392	O	MET	A	9695	68.208	49.394	59.952	1.00	15.57
1393	N	ASP	A	9796	66.113	49.992	60.504	1.00	14.90
1395	CA	ASP	A	9796	65.592	49.840	59.163	1.00	15.37
1397	CB	ASP	A	9796	64.071	49.712	59.176	1.00	15.74
1400	CG	ASP	A	9796	63.602	48.461	59.858	1.00	17.13
1401	OD1	ASP	A	9796	62.674	48.534	60.694	1.00	21.38
1402	OD2	ASP	A	9796	64.092	47.356	59.624	1.00	16.47
1403	C	ASP	A	9796	65.964	51.065	58.351	1.00	15.67
1404	O	ASP	A	9796	65.831	52.208	58.813	1.00	18.09
1405	N	GLN	A	9897	66.433	50.833	57.142	1.00	15.57
1407	CA	GLN	A	9897	66.751	51.927	56.250	1.00	15.92
1409	CB	GLN	A	9897	68.254	52.191	56.215	1.00	16.42
1412	CG	GLN	A	9897	68.986	52.134	57.542	1.00	17.34
1415	CD	GLN	A	9897	70.513	52.159	57.348	1.00	20.16
1416	OE1	GLN	A	9897	71.077	51.362	56.589	1.00	21.49
1417	NE2	GLN	A	9897	71.172	53.068	58.025	1.00	20.71
1420	C	GLN	A	9897	66.315	51.566	54.851	1.00	16.04
1421	O	GLN	A	9897	65.953	50.438	54.558	1.00	16.92
1422	N	LYS	A	9998	66.388	52.517	53.942	1.00	17.33
1424	CA	LYS	A	9998	66.011	52.179	52.589	1.00	18.24
1426	CB	LYS	A	9998	65.812	53.423	51.755	1.00	19.45
1429	CG	LYS	A	9998	66.837	54.460	51.983	1.00	24.15
1432	CD	LYS	A	9998	66.632	55.620	51.001	1.00	29.03
1435	CE	LYS	A	9998	·65.247	55.569	50.340	1.00	30.82
1438	NZ	LYS	A	9998	64.089	55.683	51.292	1.00	32.46
1442	C	LYS	A	9998	67.075	51.298	51.964	1.00	17.60
1443	O	LYS	A	9998	68.233	51.310	52.387	1.00	17.19
1444	N	CYS	A	−10099−	66.668	50.530	50.968	1.00	17.89
1446	CA	CYS	A	−10099−	67.563	49.656	50.240	1.00	18.61
1448	CB	CYS	A	−10099−	66.785	48.912	49.160	1.00	19.74
1451	SG	CYS	A	−10099−	67.861	47.885	48.131	1.00	27.28
1452	C	CYS	A	−10099−	68.660	50.466	49.582	1.00	17.61
1453	O	CYS	A	−10099−	68.362	51.409	48.851	1.00	17.91
1454	N	GLN	A	100 —101	69.919	50.123	49.846	1.00	16.17
1456	CA	GLN	A	1010	71.042	50.835	49.260	1.00	16.13
1458	CB	GLN	A	1010	71.727	51.683	50.322	1.00	16.73
1461	CG	GLN	A	1010	70.791	52.712	50.947	1.00	20.43
1464	CD	GLN	A	1010	71.229	53.147	52.329	1.00	23.94
1465	OE1	GLN	A	100-1	70.466	53.012	53.301	1.00	25.49
1466	NE2	GLN	A	1010	72.454	53.673	52.432	1.00	25.45
1469	C	GLN	A	1010	72.024	49.883	48.602	1.00	14.01
1470	O	GLN	A	1010	73.195	50.197	48.424	1.00	13.51
1471	N	TYR	A	1021	71.545	48.699	48.247	1.00	12.47
1473	CA	TYR	A	1021	72.383	47.723	47.595	1.00	12.18
1475	CB	TYR	A	1021	71.600	46.477	47.192	1.00	11.65
1478	CG	TYR	A	1021	72.451	45.520	46.371	1.00	11.45
1479	CD1	TYR	A	1021	73.403	44.707	46.961	1.00	10.07
1481	CE1	TYR	A	1021	74.173	43.863	46.246	1.00	10.60
1483	CZ	TYR	A	1021	74.082	43.836	44.874	1.00	10.34
1484	OH	TYR	A	1021	74.879	42.972	44.174	1.00	12.26

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1486	CE2	TYR	A	1021	73.155	44.636	44.265	1.00	9.92
1488	CD2	TYR	A	1021	72.372	45.474	44.994	1.00	11.91
1490	C	TYR	A	1021	73.050	48.327	46.364	1.00	12.74
1491	O	TYR	A	1021	72.405	49.007	45.560	1.00	12.69
1492	N	ASP	A	1032	74.332	48.039	46.211	1.00	12.98
1494	CA	ASP	A	1032	75.088	48.479	45.059	1.00	13.79
1496	CB	ASP	A	1032	75.903	49.703	45.437	1.00	14.41
1499	CG	ASP	A	1032	76.537	50.373	44.243	1.00	16.28
1500	OD1	ASP	A	1032	76.745	49.722	43.206	1.00	19.81
1501	OD2	ASP	A	1032	76.843	51.582	44.278	1.00	24.23
1502	C	ASP	A	1032	75.980	47.346	44.596	1.00	13.61
1503	O	ASP	A	1032	76.801	46.839	45.351	1.00	13.25
1504	N	SER	A	1043	75.835	46.914	43.349	1.00	13.73
1506	CA	SER	A	1043	76.638	45.805	42.857	1.00	14.25
1508	CB	SER	A	1043	76.175	45.382	41.481	1.00	15.37
1511	OG	SER	A	1043	76.373	46.434	40.564	1.00	18.86
1513	C	SER	A	1043	78.148	46.058	42.836	1.00	13.62
1514	O	SER	A	1043	78.933	45.111	42.780	1.00	13.57
1515	N	ALA	A	1054	78.536	47.329	42.874	1.00	14.02
1517	CA	ALA	A	1054	79.949	47.678	42.887	1.00	14.05
1519	CB	ALA	A	1054	80.114	49.188	42.778	1.00	15.04
1523	C	ALA	A	1054	80.594	47.172	44.157	1.00	14.12
1524	O	ALA	A	1054	81.811	46.993	44.212	1.00	14.91
1525	N	TYR	A	1065	79.774	46.987	45.189	1.00	12.65
1527	CA	TYR	A	1065	80.270	46.538	46.491	1.00	12.64
1529	CB	TYR	A	1065	79.717	47.432	47.584	1.00	13.67
1532	CG	TYR	A	1065	80.068	48.883	47.414	1.00	15.56
1533	CD1	TYR	A	1065	79.136	49.863	47.675	1.00	22.60
1535	CE1	TYR	A	1065	79.447	51.197	47.538	1.00	24.51
1537	CZ	TYR	A	1065	80.723	51.556	47.141	1.00	25.64
1538	OH	TYR	A	1065	81.049	52.902	47.002	1.00	30.95
1540	CE2	TYR	A	1065	81.667	50.594	46.892	1.00	23.29
1542	CD2	TYR	A	1065	81.338	49.260	47.042	1.00	19.28
1544	C	TYR	A	1065	79.924	45.080	46.801	1.00	12.60
1545	O	TYR	A	1065	80.112	44.623	47.915	1.00	12.29
1546	N	ARG	A	1076	79.675	44.286	45.780	1.00	11.59
1548	CA	ARG	A	1076	79.141	42.948	45.929	1.00	12.06
1550	CB	ARG	A	1076	78.651	42.364	44.600	1.00	12.43
1553	CG	ARG	A	1076	77.642	41.239	44.760	1.00	19.10
1556	CD	ARG	A	1076	77.714	40.157	43.714	1.00	21.47
1559	NE	ARG	A	1076	78.378	40.600	42.511	1.00	25.78
1561	CZ	ARG	A	1076	77.939	41.600	41.745	1.00	28.57
1562	NH1	ARG	A	1076	78.624	41.971	40.673	1.00	30.25
1565	NH2	ARG	A	1076	76.827	42.249	42.063	1.00	32.84
1568	C	ARG	A	1076	80.338	42.141	46.399	1.00	12.40
1569	O	ARG	A	1076	81.414	42.215	45.804	1.00	12.31
1570	N	ALA	A	1087	80.167	41.352	47.445	1.00	10.86
1572	CA	ALA	A	1087	81.228	40.480	47.924	1.00	11.36
1574	CB	ALA	A	1087	81.622	40.882	49.342	1.00	11.48
1578	C	ALA	A	1087	80.906	38.997	47.878	1.00	11.31
1579	O	ALA	A	1087	81.790	38.167	48.063	1.00	12.89

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1580	N	ALA	A	1098	79.657	38.650	47.601	1.00	10.73
1582	CA	ALA	A	1098	79.283	37.261	47.498	1.00	10.90
1584	CB	ALA	A	1098	79.051	36.650	48.879	1.00	10.89
1588	C	ALA	A	1098	78.033	37.131	46.668	1.00	10.82
1589	O	ALA	A	1098	77.316	38.101	46.463	1.00	10.40
1590	N	THR	A	11009	77.816	35.902	46.234	1.00	11.20
1592	CA	THR	A	11009	76.629	35.495	45.507	1.00	11.72
1594	CB	THR	A	11009	76.914	35.257	44.026	1.00	12.47
1596	OG1	THR	A	11009	77.961	34.278	43.875	1.00	14.50
1598	CG2	THR	A	11009	77.401	36.538	43.346	1.00	14.63
1602	C	THR	A	11009	76.154	34.217	46.144	1.00	11.75
1603	O	THR	A	11009	76.846	33.619	46.951	1.00	12.09
1604	N	CYS	A	1110	74.962	33.782	45.773	1.00	11.68
1606	CA	CYS	A	1110	74.408	32.536	46.268	1.00	11.58
1608	CB	CYS	A	1110	73.443	32.820	47.425	1.00	11.73
1611	SG	CYS	A	1110	72.680	31.361	48.109	1.00	14.24
1612	C	CYS	A	1110	73.699	31.887	45.078	1.00	11.92
1613	O	CYS	A	1110	73.008	32.601	44.340	1.00	12.45
1614	N	SER	A	1121	73.876	30.576	44.898	1.00	12.05
1616	CA	SER	A	1121	73.225	29.857	43.785	1.00	13.72
1618	CB	SER	A	1121	74.173	28.872	43.102	1.00	13.55
1621	OG	SER	A	1121	74.734	27.958	44.000	1.00	17.64
1623	C	SER	A	1121	71.971	29.142	44.236	1.00	14.06
1624	O	SER	A	1121	71.059	28.884	43.432	1.00	15.16
1625	N	LYS	A	1132	71.946	28.777	45.506	1.00	14.21
1627	CA	LYS	A	1132	70.757	28.223	46.093	1.00	14.09
1629	CB	LYS	A	1132	70.248	27.077	45.290	1.00	17.46
1632	CG	LYS	A	1132	70.764	25.827	45.665	1.00	17.84
1635	CD	LYS	A	1132	72.230	25.770	45.745	1.00	20.97
1638	CE	LYS	A	1132	72.631	24.386	45.318	1.00	24.42
1641	NZ	LYS	A	1132	71.876	23.382	46.102	1.00	26.61
1645	C	LYS	A	1132	70.976	27.866	47.545	1.00	12.54
1646	O	LYS	A	1132	72.023	28.182	48.099	1.00	11.47
1647	N	TYR	A	1143	69.974	27.275	48.169	1.00	10.94
1649	CA	TYR	A	1143	70.096	26.913	49.575	1.00	10.67
1651	CB	TYR	A	1143	69.552	28.024	50.492	1.00	9.80
1654	CG	TYR	A	1143	68.072	28.255	50.337	1.00	10.15
1655	CD1	TYR	A	1143	67.173	27.627	51.171	1.00	9.93
1657	CE1	TYR	A	1143	65.816	27.808	51.048	1.00	11.07
1659	CZ	TYR	A	1143	65.357	28.635	50.063	1.00	10.47
1660	OH	TYR	A	1143	63.979	28.824	49.933	1.00	13.05
1662	CE2	TYR	A	1143	66.216	29.291	49.237	1.00	9.92
1664	CD2	TYR	A	1143	67.588	29.105	49.368	1.00	10.20
1666	C	TYR	A	1143	69.366	25.617	49.831	1.00	10.45
1667	O	TYR	A	1143	68.549	25.174	49.023	1.00	10.52
1668	N	THR	A	1154	69.672	24.999	50.956	1.00	10.04
1670	CA	THR	A	1154	69.124	23.733	51.321	1.00	10.39
1672	CB	THR	A	1154	70.240	22.677	51.288	1.00	11.48
1674	OG1	THR	A	1154	70.762	22.562	49.953	1.00	13.46
1676	CG2	THR	A	1154	69.706	21.282	51.656	1.00	12.62
1680	C	THR	A	1154	68.589	23.835	52.724	1.00	10.67

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1681	O	THR	A	1154	69.276	24.344	53.593	1.00	11.00
1682	N	GLU	A	1165	67.381	23.353	52.940	1.00	10.19
1684	CA	GLU	A	1165	66.777	23.282	54.257	1.00	10.63
1686	CB	GLU	A	1165	65.316	23.747	54.241	1.00	11.21
1689	CG	GLU	A	1165	64.585	23.591	55.559	1.00	16.56
1692	CD	GLU	A	1165	64.938	24.657	56.577	1.00	21.26
1693	OE1	GLU	A	1165	64.685	24.415	57.762	1.00	19.91
1694	OE2	GLU	A	1165	65.429	25.737	56.194	1.00	22.35
1695	C	GLU	A	1165	66.871	21.828	54.728	1.00	10.99
1696	O	GLU	A	1165	66.487	20.899	53.992	1.00	11.77
1697	N	LEU	A	1176	67.357	21.619	55.942	1.00	9.54
1699	CA	LEU	A	1176	67.495	20.271	56.468	1.00	10.33
1701	CB	LEU	A	1176	68.592	20.261	57.529	1.00	10.13
1704	CG	LEU	A	1176	70.007	20.490	57.017	1.00	13.64
1706	CD1	LEU	A	1176	71.012	20.212	58.133	1.00	14.25
1710	CD2	LEU	A	1176	70.373	19.703	55.785	1.00	16.55
1714	C	LEU	A	1176	66.195	19.784	57.046	1.00	9.94
1715	O	LEU	A	1176	65.369	20.580	57.471	1.00	10.75
1716	N	PRO	A	1187	66.051	18.472	57.136	1.00	10.31
1717	CA	PRO	A	1187	64.820	17.889	57.653	1.00	10.41
1719	CB	PRO	A	1187	65.044	16.390	57.483	1.00	11.40
1722	CG	PRO	A	1187	66.490	16.204	57.467	1.00	13.12
1725	CD	PRO	A	1187	67.055	17.432	56.877	1.00	12.37
1728	C	PRO	A	1187	64.662	18.262	59.117	1.00	9.57
1729	O	PRO	A	1187	65.636	18.336	59.885	1.00	10.97
1730	N	TYR	A	1198	63.426	18.480	59.503	1.00	8.92
1732	CA	TYR	A	1198	63.087	18.965	60.826	1.00	8.35
1734	CB	TYR	A	1198	61.574	19.168	60.949	1.00	7.88
1737	CG	TYR	A	1198	61.190	19.665	62.313	1.00	7.93
1738	CD1	TYR	A	1198	61.126	21.015	62.577	1.00	9.08
1740	CE1	TYR	A	1198	60.824	21.472	63.814	1.00	9.37
1742	CZ	TYR	A	1198	60.588	20.603	64.837	1.00	9.28
1743	OH	TYR	A	1198	60.293	21.103	66.092	1.00	12.09
1745	CE2	TYR	A	1198	60.637	19.245	64.626	1.00	9.95
1747	CD2	TYR	A	1198	60.933	18.785	63.349	1.00	8.02
1749	C	TYR	A	1198	63.536	18.074	61.945	1.00	8.81
1750	O	TYR	A	1198	63.231	16.894	61.966	1.00	9.91
1751	N	GLY	A	12019	64.299	18.649	62.876	1.00	10.11
1753	CA	GLY	A	12019	64.647	17.981	64.108	1.00	10.48
1756	C	GLY	A	12019	65.723	16.924	64.048	1.00	10.39
1757	O	GLY	A	12019	65.980	16.279	65.061	1.00	12.29
1758	N	ARG	A	1210	66.340	16.719	62.891	1.00	10.56
1760	CA	ARG	A	1210	67.264	15.597	62.726	1.00	11.08
1762	CB	ARG	A	1210	67.163	15.021	61.318	1.00	11.64
1765	CG	ARG	A	1210	65.805	14.331	61.037	1.00	13.97
1768	CD	ARG	A	1210	65.701	12.938	61.675	1.00	18.88
1771	NE	ARG	A	1210	66.804	12.039	61.273	1.00	23.70
1773	CZ	ARG	A	1210	67.071	11.576	60.047	1.00	26.61
1774	NH1	ARG	A	1210	66.336	11.876	58.978	1.00	29.00
1777	NH2	ARG	A	1210	68.110	10.767	59.879	1.00	27.92
1780	C	ARG	A	1210	68.691	16.051	63.070	1.00	10.81

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1781	O	ARG	A	1210	69.367	16.693	62.269	1.00	10.99
1782	N	GLU	A	1221	69.172	15.658	64.238	1.00	10.92
1784	CA	GLU	A	1221	70.449	16.220	64.691	1.00	10.77
1786	CB	GLU	A	1221	70.620	16.312	66.201	1.00	11.30
1789	CG	GLU	A	1221	69.670	17.273	66.903	1.00	11.49
1792	CD	GLU	A	1221	69.914	17.279	68.383	1.00	10.90
1793	OE1	GLU	A	1221	70.907	17.924	68.809	1.00	12.61
1794	OE2	GLU	A	1221	69.158	16.617	69.113	1.00	12.77
1795	C	GLU	A	1221	71.587	15.480	64.025	1.00	10.70
1796	O	GLU	A	1221	72.685	16.019	63.883	1.00	10.04
1797	N	ASP	A	1232	71.319	14.245	63.611	1.00	11.23
1799	CA	ASP	A	1232	72.294	13.496	62.832	1.00	11.54
1801	CB	ASP	A	1232	71.919	12.004	62.746	1.00	12.35
1804	CG	ASP	A	1232	70.522	11.758	62.259	1.00	16.29
1805	OD1	ASP	A	1232	70.224	10.549	62.035	1.00	23.03
1806	OD2	ASP	A	1232	69.645	12.629	62.091	1.00	17.22
1807	C	ASP	A	1232	72.546	14.105	61.444	1.00	10.74
1808	O	ASP	A	1232	73.690	14.193	60.962	1.00	11.34
1809	N	VAL	A	1243	71.481	14.561	60.798	1.00	10.66
1811	CA	VAL	A	1243	71.609	15.201	59.509	1.00	10.45
1813	CB	VAL	A	1243	70.233	15.362	58.831	1.00	10.68
1815	CG1	VAL	A	1243	70.379	16.127	57.531	1.00	11.63
1819	CG2	VAL	A	1243	69.605	13.981	58.619	1.00	12.29
1823	C	VAL	A	1243	72.314	16.552	59.671	1.00	9.04
1824	O	VAL	A	1243	73.123	16.944	58.838	1.00	10.27
1825	N	LEU	A	1254	71.999	17.263	60.759	1.00	9.71
1827	CA	LEU	A	1254	72.655	18.523	61.022	1.00	8.77
1829	CB	LEU	A	1254	72.002	19.215	62.216	1.00	8.25
1832	CG	LEU	A	1254	72.631	20.545	62.603	1.00	8.58
1834	CD1	LEU	A	1254	72.640	21.547	61.459	1.00	7.65
1838	CD2	LEU	A	1254	71.956	21.115	63.819	1.00	8.88
1842	C	LEU	A	1254	74.144	18.295	61.231	1.00	8.32
1843	O	LEU	A	1254	74.958	19.040	60.720	1.00	8.40
1844	N	LYS	A	1265	74.488	17.221	61.933	1.00	9.47
1846	CA	LYS	A	1265	75.884	16.902	62.181	1.00	9.80
1848	CB	LYS	A	1265	75.982	15.710	63.116	1.00	10.35
1851	CG	LYS	A	1265	77.422	15.326	63.446	1.00	11.29
1854	CD	LYS	A	1265	77.496	14.014	64.157	1.00	11.93
1857	CE	LYS	A	1265	78.932	13.613	64.384	1.00	14.42
1860	NZ	LYS	A	1265	79.002	12.244	65.003	1.00	14.97
1864	C	LYS	A	1265	76.632	16.645	60.878	1.00	10.19
1865	O	LYS	A	1265	77.689	17.168	60.618	1.00	9.36
1866	N	GLU	A	1276	75.940	16.060	59.934	1.00	10.68
1868	CA	GLU	A	1276	76.528	15.618	58.698	1.00	11.80
1870	CB	GLU	A	1276	75.581	14.703	57.924	1.00	12.26
1873	CG	GLU	A	1276	76.183	14.184	56.625	1.00	17.82
1876	CD	GLU	A	1276	75.249	13.231	55.880	1.00	24.81
1877	OE1	GLU	A	1276	75.594	12.820	54.748	1.00	30.58
1878	OE2	GLU	A	1276	74.169	12.878	56.415	1.00	30.81
1879	C	GLU	A	1276	76.765	16.890	57.886	1.00	10.63
1880	O	GLU	A	1276	77.803	17.063	57.261	1.00	10.41

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1881	N	ALA	A	128~~7~~	75.802	17.802	57.919	1.00	9.65
1883	CA	ALA	A	128~~7~~	75.906	19.038	57.162	1.00	9.46
1885	CB	ALA	A	128~~7~~	74.572	19.791	57.174	1.00	9.65
1889	C	ALA	A	128~~7~~	77.026	19.929	57.705	1.00	9.71
1890	O	ALA	A	128~~7~~	77.773	20.557	56.966	1.00	8.97
1891	N	VAL	A	129~~8~~	77.104	20.009	59.024	1.00	9.81
1893	CA	VAL	A	129~~8~~	78.131	20.834	59.641	1.00	10.35
1895	CB	VAL	A	129~~8~~	77.932	20.917	61.164	1.00	9.67
1897	CG1	VAL	A	129~~8~~	79.111	21.636	61.831	1.00	10.09
1901	CG2	VAL	A	129~~8~~	76.657	21.658	61.498	1.00	11.58
1905	C	VAL	A	129~~8~~	79.512	20.257	59.304	1.00	10.25
1906	O	VAL	A	129~~8~~	80.451	21.011	58.991	1.00	11.60
1907	N	ALA	A	130~~29~~	79.635	18.931	59.303	1.00	10.33
1909	CA	ALA	A	130~~29~~	80.921	18.297	58.986	1.00	10.92
1911	CB	ALA	A	130~~29~~	80.887	16.835	59.372	1.00	11.58
1915	C	ALA	A	130~~29~~	81.320	18.420	57.512	1.00	11.52
1916	O	ALA	A	130~~29~~	82.473	18.681	57.169	1.00	13.47
1917	N	ASN	A	131~~0~~	80.328	18.230	56.647	1.00	12.06
1919	CA	ASN	A	131~~0~~	80.564	18.098	55.216	1.00	12.89
1921	CB	ASN	A	131~~0~~	79.779	16.903	54.697	1.00	13.41
1924	CG	ASN	A	131~~0~~	80.098	15.642	55.462	1.00	18.03
1925	OD1	ASN	A	131~~0~~	81.175	15.529	56.058	1.00	23.95
1926	ND2	ASN	A	131~~0~~	79.162	14.685	55.468	1.00	24.96
1929	C	ASN	A	131~~0~~	80.265	19.299	54.346	1.00	12.52
1930	O	ASN	A	131~~0~~	80.785	19.386	53.224	1.00	14.05
1931	N	LYS	A	132~~1~~	79.447	20.219	54.828	1.00	11.98
1933	CA	LYS	A	132~~1~~	79.047	21.379	54.034	1.00	11.52
1935	CB	LYS	A	132~~1~~	77.523	21.475	53.903	1.00	12.09
1938	CG	LYS	A	132~~1~~	76.879	20.234	53.333	1.00	14.86
1941	CD	LYS	A	132~~1~~	77.338	19.976	51.948	1.00	18.60
1944	CE	LYS	A	132~~1~~	76.628	18.765	51.370	1.00	22.39
1947	NZ	LYS	A	132~~1~~	77.040	18.566	49.974	1.00	24.93
1951	C	LYS	A	132~~1~~	79.579	22.672	54.618	1.00	10.89
1952	O	LYS	A	132~~1~~	80.044	23.511	53.890	1.00	12.16
1953	N	GLY	A	133~~2~~	79.509	22.825	55.933	1.00	10.86
1955	CA	GLY	A	133~~2~~	80.018	24.022	56.574	1.00	10.39
1958	C	GLY	A	133~~2~~	79.024	24.471	57.621	1.00	9.08
1959	O	GLY	A	133~~2~~	78.100	23.754	57.957	1.00	9.22
1960	N	PRO	A	134~~3~~	79.237	25.667	58.151	1.00	8.54
1961	CA	PRO	A	134~~3~~	78.321	26.231	59.126	1.00	8.52
1963	CB	PRO	A	134~~3~~	78.898	27.624	59.367	1.00	8.68
1966	CG	PRO	A	134~~3~~	80.386	27.413	59.170	1.00	8.71
1969	CD	PRO	A	134~~3~~	80.400	26.527	57.936	1.00	8.56
1972	C	PRO	A	134~~3~~	76.890	26.293	58.605	1.00	8.18
1973	O	PRO	A	134~~3~~	76.646	26.564	57.423	1.00	9.37
1974	N	VAL	A	135~~4~~	75.958	26.069	59.519	1.00	7.77
1976	CA	VAL	A	135~~4~~	74.552	25.970	59.171	1.00	7.23
1978	CB	VAL	A	135~~4~~	74.013	24.564	59.455	1.00	7.86
1980	CG1	VAL	A	135~~4~~	72.528	24.473	59.155	1.00	7.98
1984	CG2	VAL	A	135~~4~~	74.793	23.524	58.652	1.00	9.33
1988	C	VAL	A	135~~4~~	73.724	26.964	59.948	1.00	7.50

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
1989	O	VAL	A	1354	73.855	27.053	61.166	1.00	7.45
1990	N	SER	A	1365	72.879	27.701	59.261	1.00	6.93
1992	CA	SER	A	1365	71.992	28.640	59.914	1.00	6.89
1994	CB	SER	A	1365	71.336	29.558	58.896	1.00	7.58
1997	OG	SER	A	1365	72.280	30.389	58.274	1.00	9.26
1999	C	SER	A	1365	70.904	27.873	60.625	1.00	7.76
2000	O	SER	A	1365	70.312	26.979	60.050	1.00	8.27
2001	N	VAL	A	1376	70.608	28.229	61.861	1.00	6.95
2003	CA	VAL	A	1376	69.553	27.579	62.604	1.00	7.33
2005	CB	VAL	A	1376	70.106	26.481	63.549	1.00	7.43
2007	CG1	VAL	A	1376	70.796	25.365	62.779	1.00	7.54
2011	CG2	VAL	A	1376	71.018	27.098	64.582	1.00	8.98
2015	C	VAL	A	1376	68.798	28.565	63.453	1.00	7.01
2016	O	VAL	A	1376	69.272	29.670	63.673	1.00	7.91
2017	N	GLY	A	1387	67.632	28.155	63.930	1.00	7.99
2019	CA	GLY	A	1387	66.915	28.927	64.927	1.00	8.21
2022	C	GLY	A	1387	66.959	28.190	66.241	1.00	8.99
2023	O	GLY	A	1387	66.969	26.950	66.266	1.00	10.44
2024	N	VAL	A	1398	66.994	28.945	67.335	1.00	8.90
2026	CA	VAL	A	1398	66.934	28.357	68.646	1.00	8.49
2028	CB	VAL	A	1398	68.301	28.366	69.380	1.00	9.11
2030	CG1	VAL	A	1398	69.303	27.488	68.667	1.00	10.12
2034	CG2	VAL	A	1398	68.809	29.787	69.552	1.00	10.01
2038	C	VAL	A	1398	65.915	29.113	69.470	1.00	8.74
2039	O	VAL	A	1398	65.580	30.261	69.168	1.00	9.27
2040	N	ASP	A	14039	65.439	28.453	70.515	1.00	9.41
2042	CA	ASP	A	14039	64.619	29.080	71.532	1.00	9.75
2044	CB	ASP	A	14039	63.758	28.027	72.221	1.00	10.36
2047	CG	ASP	A	14039	62.973	28.567	73.382	1.00	13.95
2048	OD1	ASP	A	14039	63.018	29.788	73.636	1.00	13.07
2049	OD2	ASP	A	14039	62.280	27.821	74.089	1.00	12.63
2050	C	ASP	A	14039	65.582	29.742	72.509	1.00	10.48
2051	O	ASP	A	14039	66.192	29.070	73.340	1.00	11.23
2052	N	ALA	A	1410	65.736	31.055	72.376	1.00	9.84
2054	CA	ALA	A	1410	66.627	31.800	73.255	1.00	10.56
2056	CB	ALA	A	1410	67.563	32.644	72.403	1.00	10.21
2060	C	ALA	A	1410	65.864	32.696	74.230	1.00	11.65
2061	O	ALA	A	1410	66.420	33.703	74.660	1.00	13.88
2062	N	ALA	A	1421	64.618	32.340	74.559	1.00	11.62
2064	CA	ALA	A	1421	63.701	33.170	75.383	1.00	12.34
2066	CB	ALA	A	1421	62.279	32.790	75.045	1.00	13.28
2070	C	ALA	A	1421	63.848	33.075	76.893	1.00	12.91
2071	O	ALA	A	1421	63.299	33.897	77.640	1.00	14.20
2072	N	HIS	A	1432	64.542	32.028	77.328	1.00	11.67
2074	CA	HIS	A	1432	64.734	31.745	78.736	1.00	10.65
2076	CB	HIS	A	1432	64.909	30.229	78.886	1.00	11.31
2079	CG	HIS	A	1432	63.760	29.489	78.294	1.00	12.62
2080	ND1	HIS	A	1432	62.563	29.392	78.958	1.00	15.67
2082	CE1	HIS	A	1432	61.677	28.789	78.187	1.00	18.84
2084	NE2	HIS	A	1432	62.233	28.582	77.012	1.00	17.98
2086	CD2	HIS	A	1432	63.541	28.995	77.055	1.00	16.74

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2088	C	HIS	A	1432	65.867	32.533	79.375	1.00	10.05
2089	O	HIS	A	1432	66.957	32.677	78.813	1.00	8.85
2090	N	PRO	A	1443	65.618	33.058	80.572	1.00	9.31
2091	CA	PRO	A	1443	66.619	33.858	81.263	1.00	9.10
2093	CB	PRO	A	1443	65.981	34.078	82.639	1.00	9.27
2096	CG	PRO	A	1443	64.554	34.116	82.356	1.00	9.48
2099	CD	PRO	A	1443	64.356	33.003	81.328	1.00	10.45
2102	C	PRO	A	1443	68.002	33.226	81.356	1.00	9.20
2103	O	PRO	A	1443	69.002	33.922	81.269	1.00	9.58
2104	N	SER	A	1454	68.074	31.912	81.469	1.00	8.53
2106	CA	SER	A	1454	69.355	31.241	81.507	1.00	9.24
2108	CB	SER	A	1454	69.181	29.741	81.708	1.00	9.98
2111	OG	SER	A	1454	68.353	29.206	80.689	1.00	10.17
2113	C	SER	A	1454	70.195	31.442	80.252	1.00	9.24
2114	O	SER	A	1454	71.404	31.438	80.302	1.00	10.26
2115	N	PHE	A	1465	69.550	31.622	79.120	1.00	8.12
2117	CA	PHE	A	1465	70.280	31.777	77.878	1.00	8.41
2119	CB	PHE	A	1465	69.311	31.790	76.696	1.00	8.68
2122	CG	PHE	A	1465	69.989	31.730	75.353	1.00	9.31
2123	CD1	PHE	A	1465	70.446	32.864	74.738	1.00	9.11
2125	CE1	PHE	A	1465	71.073	32.815	73.499	1.00	10.41
2127	CZ	PHE	A	1465	71.237	31.604	72.858	1.00	8.98
2129	CE2	PHE	A	1465	70.784	30.463	73.447	1.00	9.09
2131	CD2	PHE	A	1465	70.168	30.514	74.713	1.00	9.83
2133	C	PHE	A	1465	71.099	33.051	77.918	1.00	8.58
2134	O	PHE	A	1465	72.256	33.075	77.535	1.00	8.66
2135	N	PHE	A	1476	70.463	34.134	78.344	1.00	8.28
2137	CA	PHE	A	1476	71.145	35.416	78.385	1.00	8.90
2139	CB	PHE	A	1476	70.175	36.519	78.836	1.00	8.80
2142	CG	PHE	A	1476	68.910	36.602	78.030	1.00	9.02
2143	CD1	PHE	A	1476	68.874	37.264	76.829	1.00	10.28
2145	CE1	PHE	A	1476	67.695	37.367	76.112	1.00	11.17
2147	CZ	PHE	A	1476	66.559	36.771	76.579	1.00	11.26
2149	CE2	PHE	A	1476	66.588	36.141	77.766	1.00	10.27
2151	CD2	PHE	A	1476	67.742	36.050	78.496	1.00	11.76
2153	C	PHE	A	1476	72.332	35.409	79.336	1.00	8.96
2154	O	PHE	A	1476	73.280	36.161	79.153	1.00	9.91
2155	N	LEU	A	1487	72.257	34.562	80.357	1.00	8.62
2157	CA	LEU	A	1487	73.269	34.494	81.405	1.00	8.80
2159	CB	LEU	A	1487	72.587	34.268	82.750	1.00	9.36
2162	CG	LEU	A	1487	71.784	35.450	83.268	1.00	11.87
2164	CD1	LEU	A	1487	70.837	35.007	84.357	1.00	13.02
2168	CD2	LEU	A	1487	72.709	36.549	83.731	1.00	14.79
2172	C	LEU	A	1487	74.315	33.419	81.194	1.00	8.48
2173	O	LEU	A	1487	75.194	33.203	82.040	1.00	8.85
2174	N	TYR	A	1498	74.251	32.723	80.068	1.00	8.43
2176	CA	TYR	A	1498	75.216	31.682	79.795	1.00	8.84
2178	CB	TYR	A	1498	74.903	31.084	78.413	1.00	9.11
2181	CG	TYR	A	1498	75.998	30.135	77.957	1.00	8.12
2182	CD1	TYR	A	1498	77.085	30.588	77.249	1.00	10.58
2184	CE1	TYR	A	1498	78.093	29.724	76.861	1.00	10.61

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2186	CZ	TYR	A	149̶8̶	78.030	28.432	77.211	1.00	10.21
2187	OH	TYR	A	149̶8̶	79.002	27.527	76.847	1.00	12.73
2189	CE2	TYR	A	149̶8̶	76.973	27.949	77.918	1.00	8.84
2191	CD2	TYR	A	149̶8̶	75.974	28.812	78.316	1.00	8.14
2193	C	TYR	A	149̶8̶	76.630	32.239	79.786	1.00	9.36
2194	O	TYR	A	149̶8̶	76.894	33.240	79.156	1.00	9.91
2195	N	ARG	A	150̶4̶9̶	77.562	31.475	80.337	1.00	11.00
2197	CA	ARG	A	150̶4̶9̶	78.940	31.916	80.410	1.00	13.06
2199	CB	ARG	A	150̶4̶9̶	79.383	32.296	81.818	1.00	13.71
2202	CG	ARG	A	150̶4̶9̶	78.785	33.579	82.319	1.00	17.64
2205	CD	ARG	A	150̶4̶9̶	79.526	34.139	83.521	1.00	22.44
2208	NE	ARG	A	150̶4̶9̶	80.525	35.139	83.150	1.00	28.55
2210	CZ	ARG	A	150̶4̶9̶	81.330	35.754	84.011	1.00	29.06
2211	NH1	ARG	A	150̶4̶9̶	81.275	35.466	85.315	1.00	32.76
2214	NH2	ARG	A	150̶4̶9̶	82.212	36.646	83.566	1.00	32.91
2217	C	ARG	A	150̶4̶9̶	79.847	30.859	79.853	1.00	14.38
2218	O	ARG	A	150̶4̶9̶	80.711	31.177	79.051	1.00	16.28
2219	N	SER	A	151̶0̶	79.635	29.623	80.254	1.00	14.09
2221	CA	SER	A	151̶0̶	80.498	28.530	79.838	1.00	15.27
2223	CB	SER	A	151̶0̶	81.763	28.574	80.702	1.00	16.19
2226	OG	SER	A	151̶0̶	81.422	28.217	82.023	1.00	20.80
2228	C	SER	A	151̶0̶	79.841	27.175	80.004	1.00	13.74
2229	O	SER	A	151̶0̶	78.766	27.039	80.535	1.00	14.33
2230	N	GLY	A	152̶1̶	80.513	26.140	79.519	1.00	14.22
2232	CA	GLY	A	152̶1̶	79.983	24.808	79.634	1.00	13.52
2235	C	GLY	A	152̶1̶	78.998	24.506	78.519	1.00	12.08
2236	O	GLY	A	152̶1̶	78.956	25.171	77.499	1.00	13.44
2237	N	VAL	A	153̶2̶	78.205	23.482	78.735	1.00	10.92
2239	CA	VAL	A	153̶2̶	77.216	23.103	77.735	1.00	10.45
2241	CB	VAL	A	153̶2̶	77.243	21.614	77.462	1.00	9.54
2243	CG1	VAL	A	153̶2̶	76.052	21.211	76.602	1.00	12.64
2247	CG2	VAL	A	153̶2̶	78.545	21.268	76.795	1.00	10.69
2251	C	VAL	A	153̶2̶	75.857	23.493	78.243	1.00	10.27
2252	O	VAL	A	153̶2̶	75.387	23.015	79.278	1.00	12.04
2253	N	TYR	A	154̶3̶	75.198	24.361	77.495	1.00	9.96
2255	CA	TYR	A	154̶3̶	73.890	24.856	77.873	1.00	9.51
2257	CB	TYR	A	154̶3̶	73.513	26.043	77.003	1.00	9.63
2260	CG	TYR	A	154̶3̶	72.192	26.721	77.327	1.00	7.69
2261	CD1	TYR	A	154̶3̶	72.065	27.565	78.410	1.00	9.40
2263	CE1	TYR	A	154̶3̶	70.891	28.185	78.667	1.00	8.73
2265	CZ	TYR	A	154̶3̶	69.809	27.993	77.857	1.00	9.00
2266	OH	TYR	A	154̶3̶	68.624	28.620	78.089	1.00	9.78
2268	CE2	TYR	A	154̶3̶	69.894	27.172	76.783	1.00	10.21
2270	CD2	TYR	A	154̶3̶	71.083	26.549	76.511	1.00	9.56
2272	C	TYR	A	154̶3̶	72.798	23.809	77.749	1.00	10.46
2273	O	TYR	A	154̶3̶	72.546	23.248	76.683	1.00	10.19
2274	N	TYR	A	155̶4̶	72.137	23.545	78.858	1.00	11.08
2276	CA	TYR	A	155̶4̶	70.962	22.703	78.890	1.00	11.49
2278	CB	TYR	A	155̶4̶	71.261	21.291	79.366	1.00	11.90
2281	CG	TYR	A	155̶4̶	70.029	20.416	79.355	1.00	13.97
2282	CD1	TYR	A	155̶4̶	69.609	19.792	78.188	1.00	16.03

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2284	CE1	TYR	A	1554	68.479	19.018	78.160	1.00	17.16
2286	CZ	TYR	A	1554	67.755	18.855	79.317	1.00	19.32
2287	OH	TYR	A	1554	66.627	18.085	79.327	1.00	21.76
2289	CE2	TYR	A	1554	68.148	19.459	80.480	1.00	18.42
2291	CD2	TYR	A	1554	69.270	20.239	80.497	1.00	16.68
2293	C	TYR	A	1554	69.948	23.378	79.803	1.00	12.53
2294	O	TYR	A	1554	70.248	23.643	80.971	1.00	12.82
2295	N	GLU	A	1565	68.775	23.664	79.264	1.00	11.20
2297	CA	GLU	A	1565	67.724	24.357	79.989	1.00	12.03
2299	CB	GLU	A	1565	67.501	25.714	79.326	1.00	12.58
2302	CG	GLU	A	1565	66.272	26.509	79.780	1.00	13.48
2305	CD	GLU	A	1565	66.192	26.623	81.281	1.00	15.11
2306	OE1	GLU	A	1565	66.809	27.561	81.860	1.00	15.68
2307	OE2	GLU	A	1565	65.542	25.771	81.919	1.00	15.92
2308	C	GLU	A	1565	66.473	23.486	79.900	1.00	12.76
2309	O	GLU	A	1565	65.887	23.384	78.845	1.00	12.36
2310	N	PRO	A	1576	66.080	22.870	81.015	1.00	13.89
2311	CA	PRO	A	1576	64.876	22.036	81.084	1.00	15.01
2313	CB	PRO	A	1576	64.714	21.783	82.585	1.00	15.26
2316	CG	PRO	A	1576	66.057	21.897	83.121	1.00	15.94
2319	CD	PRO	A	1576	66.809	22.891	82.288	1.00	14.46
2322	C	PRO	A	1576	63.639	22.726	80.555	1.00	15.21
2323	O	PRO	A	1576	62.798	22.051	79.979	1.00	16.52
2324	N	SER	A	1587	63.534	24.037	80.704	1.00	15.00
2326	CA	SER	A	1587	62.360	24.768	80.231	1.00	15.20
2328	CB	SER	A	1587	62.195	26.054	81.040	1.00	15.85
2331	OG	SER	A	1587	63.200	27.009	80.694	1.00	18.36
2333	C	SER	A	1587	62.395	25.112	78.739	1.00	15.01
2334	O	SER	A	1587	61.444	25.698	78.195	1.00	14.99
2335	N	CYS	A	1598	63.479	24.765	78.058	1.00	14.65
2337	CA	CYS	A	1598	63.576	25.121	76.659	1.00	15.32
2339	CB	CYS	A	1598	64.971	24.807	76.111	1.00	15.82
2342	SG	CYS	A	1598	65.717	26.157	75.134	1.00	19.46
2343	C	CYS	A	1598	62.506	24.363	75.865	1.00	15.27
2344	O	CYS	A	1598	61.992	23.325	76.303	1.00	16.56
2345	N	THR	A	16059	62.196	24.894	74.691	1.00	14.37
2347	CA	THR	A	16059	61.195	24.313	73.800	1.00	14.29
2349	CB	THR	A	16059	59.929	25.174	73.781	1.00	15.27
2351	OG1	THR	A	16059	60.186	26.373	73.034	1.00	15.16
2353	CG2	THR	A	16059	59.555	25.644	75.163	1.00	15.70
2357	C	THR	A	16059	61.739	24.279	72.400	1.00	13.99
2358	O	THR	A	16059	62.850	24.736	72.134	1.00	13.31
2359	N	GLN	A	1610	60.916	23.758	71.490	1.00	13.08
2361	CA	GLN	A	1610	61.240	23.746	70.090	1.00	13.25
2363	CB	GLN	A	1610	60.896	22.388	69.467	1.00	13.15
2366	CG	GLN	A	1610	61.858	21.270	69.856	1.00	12.98
2369	CD	GLN	A	1610	61.565	20.677	71.210	1.00	13.59
2370	OE1	GLN	A	1610	60.429	20.644	71.657	1.00	14.17
2371	NE2	GLN	A	1610	62.615	20.193	71.884	1.00	15.01
2374	C	GLN	A	1610	60.533	24.906	69.372	1.00	13.83
2375	O	GLN	A	1610	60.429	24.913	68.152	1.00	15.62

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2376	N	ASN	A	162~~1~~	60.080	25.897	70.127	1.00	14.74
2378	CA	ASN	A	162~~1~~	59.421	27.067	69.564	1.00	15.59
2380	CB	ASN	A	162~~1~~	58.341	27.560	70.512	1.00	16.23
2383	CG	ASN	A	162~~1~~	57.219	26.544	70.671	1.00	19.55
2384	OD1	ASN	A	162~~1~~	56.731	25.975	69.673	1.00	23.25
2385	ND2	ASN	A	162~~1~~	56.819	26.293	71.904	1.00	24.33
2388	C	ASN	A	162~~1~~	60.465	28.140	69.298	1.00	15.36
2389	O	ASN	A	162~~1~~	60.998	28.734	70.219	1.00	15.41
2390	N	VAL	A	163~~2~~	61.244	28.131	68.187	1.00	10.65
2392	CA	VAL	A	163~~2~~	62.485	28.881	68.008	1.00	10.29
2394	CB	VAL	A	163~~2~~	63.377	28.307	66.901	1.00	10.87
2396	CG1	VAL	A	163~~2~~	63.729	26.861	67.248	1.00	12.53
2400	CG2	VAL	A	163~~2~~	62.717	28.419	65.514	1.00	12.13
2404	C	VAL	A	163~~2~~	62.164	30.342	67.757	1.00	10.71
2405	O	VAL	A	163~~2~~	61.155	30.657	67.136	1.00	12.16
2406	N	ASN	A	164~~3~~	63.039	31.227	68.213	1.00	9.91
2408	CA	ASN	A	164~~3~~	62.806	32.652	68.074	1.00	10.63
2410	CB	ASN	A	164~~3~~	62.208	33.229	69.355	1.00	10.42
2413	CG	ASN	A	164~~3~~	63.244	33.413	70.465	1.00	13.48
2414	OD1	ASN	A	164~~3~~	64.071	32.579	70.671	1.00	12.41
2415	ND2	ASN	A	164~~3~~	63.180	34.555	71.186	1.00	19.14
2418	C	ASN	A	164~~3~~	64.045	33.427	67.692	1.00	9.92
2419	O	ASN	A	164~~3~~	63.965	34.638	67.463	1.00	11.88
2420	N	HIS	A	165~~4~~	65.191	32.767	67.602	1.00	8.50
2422	CA	HIS	A	165~~4~~	66.438	33.483	67.417	1.00	8.73
2424	CB	HIS	A	165~~4~~	67.081	33.581	68.793	1.00	8.53
2427	CG	HIS	A	165~~4~~	68.328	34.386	68.828	1.00	9.08
2428	ND1	HIS	A	165~~4~~	68.371	35.704	68.410	1.00	14.10
2430	CE1	HIS	A	165~~4~~	69.597	36.171	68.592	1.00	14.09
2432	NE2	HIS	A	165~~4~~	70.331	35.218	69.142	1.00	11.57
2434	CD2	HIS	A	165~~4~~	69.555	34.099	69.311	1.00	11.96
2436	C	HIS	A	165~~4~~	67.370	32.780	66.434	1.00	8.56
2437	O	HIS	A	165~~4~~	67.745	31.614	66.634	1.00	9.41
2438	N	GLY	A	166~~5~~	67.717	33.467	65.374	1.00	7.36
2440	CA	GLY	A	166~~5~~	68.592	32.911	64.370	1.00	7.82
2443	C	GLY	A	166~~5~~	70.032	32.978	64.818	1.00	7.99
2444	O	GLY	A	166~~5~~	70.501	34.036	65.242	1.00	9.99
2445	N	VAL	A	167~~6~~	70.744	31.866	64.694	1.00	7.36
2447	CA	VAL	A	167~~6~~	72.145	31.790	65.058	1.00	7.23
2449	CB	VAL	A	167~~6~~	72.330	31.254	66.486	1.00	7.45
2451	CG1	VAL	A	167~~6~~	71.776	32.242	67.496	1.00	10.34
2455	CG2	VAL	A	167~~6~~	71.703	29.909	66.652	1.00	7.32
2459	C	VAL	A	167~~6~~	72.853	30.900	64.042	1.00	7.36
2460	O	VAL	A	167~~6~~	72.233	30.459	63.065	1.00	7.38
2461	N	LEU	A	168~~7~~	74.135	30.625	64.247	1.00	6.74
2463	CA	LEU	A	168~~7~~	74.915	29.864	63.302	1.00	6.96
2465	CB	LEU	A	168~~7~~	75.923	30.780	62.614	1.00	7.61
2468	CG	LEU	A	168~~7~~	76.767	30.201	61.496	1.00	7.59
2470	CD1	LEU	A	168~~7~~	75.862	29.930	60.278	1.00	8.89
2474	CD2	LEU	A	168~~7~~	77.897	31.107	61.118	1.00	9.51
2478	C	LEU	A	168~~7~~	75.630	28.753	64.011	1.00	7.40

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2479	O	LEU	A	1687	76.400	29.003	64.947	1.00	8.25
2480	N	VAL	A	1698	75.394	27.541	63.559	1.00	6.97
2482	CA	VAL	A	1698	76.115	26.392	64.075	1.00	7.43
2484	CB	VAL	A	1698	75.348	25.099	63.926	1.00	8.17
2486	CG1	VAL	A	1698	76.236	23.950	64.379	1.00	7.39
2490	CG2	VAL	A	1698	74.059	25.167	64.691	1.00	8.53
2494	C	VAL	A	1698	77.425	26.302	63.324	1.00	8.18
2495	O	VAL	A	1698	77.448	26.068	62.100	1.00	9.10
2496	N	VAL	A	17069	78.543	26.455	64.034	1.00	8.35
2498	CA	VAL	A	17069	79.851	26.441	63.420	1.00	8.74
2500	CB	VAL	A	17069	80.664	27.719	63.735	1.00	8.05
2502	CG1	VAL	A	17069	79.982	28.943	63.129	1.00	9.46
2506	CG2	VAL	A	17069	80.809	27.912	65.233	1.00	10.17
2510	C	VAL	A	17069	80.662	25.216	63.815	1.00	8.49
2511	O	VAL	A	17069	81.825	25.106	63.451	1.00	10.30
2512	N	GLY	A	1710	80.062	24.296	64.544	1.00	7.21
2514	CA	GLY	A	1710	80.774	23.110	64.936	1.00	8.40
2517	C	GLY	A	1710	79.981	22.284	65.906	1.00	8.29
2518	O	GLY	A	1710	78.808	22.542	66.190	1.00	8.22
2519	N	TYR	A	1721	80.629	21.254	66.434	1.00	8.01
2521	CA	TYR	A	1721	80.011	20.367	67.390	1.00	7.80
2523	CB	TYR	A	1721	79.006	19.427	66.709	1.00	8.02
2526	CG	TYR	A	1721	79.592	18.493	65.663	1.00	8.30
2527	CD1	TYR	A	1721	80.284	17.361	66.027	1.00	8.34
2529	CE1	TYR	A	1721	80.815	16.518	65.075	1.00	8.68
2531	CZ	TYR	A	1721	80.618	16.792	63.747	1.00	9.96
2532	OH	TYR	A	1721	81.121	15.957	62.775	1.00	11.55
2534	CE2	TYR	A	1721	79.912	17.876	63.360	1.00	8.86
2536	CD2	TYR	A	1721	79.413	18.734	64.302	1.00	7.83
2538	C	TYR	A	1721	81.136	19.597	68.046	1.00	8.93
2539	O	TYR	A	1721	82.249	19.563	67.543	1.00	8.28
2540	N	GLY	A	1732	80.834	19.004	69.172	1.00	8.40
2542	CA	GLY	A	1732	81.820	18.201	69.876	1.00	9.34
2545	C	GLY	A	1732	81.264	17.659	71.165	1.00	10.09
2546	O	GLY	A	1732	80.067	17.484	71.341	1.00	9.49
2547	N	ASP	A	1743	82.175	17.379	72.104	1.00	10.45
2549	CA	ASP	A	1743	81.818	16.824	73.403	1.00	12.07
2551	CB	ASP	A	1743	82.013	15.300	73.436	1.00	13.42
2554	CG	ASP	A	1743	81.284	14.610	74.585	1.00	19.33
2555	OD1	ASP	A	1743	81.207	13.357	74.509	1.00	28.93
2556	OD2	ASP	A	1743	80.778	15.185	75.585	1.00	27.58
2557	C	ASP	A	1743	82.709	17.469	74.437	1.00	10.98
2558	O	ASP	A	1743	83.919	17.569	74.232	1.00	11.78
2559	N	LEU	A	1754	82.067	17.967	75.488	1.00	10.40
2561	CA	LEU	A	1754	82.717	18.587	76.620	1.00	10.52
2563	CB	LEU	A	1754	82.469	20.086	76.644	1.00	10.62
2566	CG	LEU	A	1754	83.006	20.880	77.849	1.00	12.27
2568	CD1	LEU	A	1754	84.506	20.809	78.011	1.00	12.13
2572	CD2	LEU	A	1754	82.555	22.308	77.817	1.00	12.39
2576	C	LEU	A	1754	82.218	17.963	77.915	1.00	10.70
2578	N	ASN	A	1765	83.244	17.305	78.488	1.00	11.40

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2580	CA	ASN	A	1765	83.055	16.651	79.768	1.00	12.77
2582	CB	ASN	A	1765	82.958	17.689	80.875	1.00	12.71
2585	CG	ASN	A	1765	84.244	18.472	81.011	1.00	12.93
2586	OD1	ASN	A	1765	84.246	19.699	81.145	1.00	17.26
2587	ND2	ASN	A	1765	85.337	17.769	80.953	1.00	12.62
2590	C	ASN	A	1765	81.853	15.742	79.772	1.00	13.51
2591	O	ASN	A	1765	81.044	15.776	80.695	1.00	14.67
2592	N	GLY	A	1776	81.762	14.911	78.751	1.00	15.00
2594	CA	GLY	A	1776	80.671	13.965	78.665	1.00	15.11
2597	C	GLY	A	1776	79.423	14.498	77.988	1.00	14.77
2598	O	GLY	A	1776	78.552	13.727	77.590	1.00	17.38
2599	N	LYS	A	1787	79.339	15.813	77.811	1.00	13.42
2601	CA	LYS	A	1787	78.161	16.434	77.204	1.00	12.76
2603	CB	LYS	A	1787	77.758	17.674	77.987	1.00	13.18
2606	CG	LYS	A	1787	77.487	17.411	79.472	1.00	14.98
2609	CD	LYS	A	1787	76.298	16.494	79.681	1.00	18.24
2612	CE	LYS	A	1787	75.904	16.428	81.139	1.00	21.11
2615	NZ	LYS	A	1787	74.698	15.565	81.266	1.00	22.91
2619	C	LYS	A	1787	78.387	16.817	75.744	1.00	11.44
2620	O	LYS	A	1787	79.223	17.660	75.441	1.00	10.83
2621	N	GLU	A	1798	77.608	16.224	74.839	1.00	10.74
2623	CA	GLU	A	1798	77.712	16.577	73.444	1.00	10.50
2625	CB	GLU	A	1798	76.946	15.580	72.603	1.00	11.29
2628	CG	GLU	A	1798	77.486	14.178	72.767	1.00	13.43
2631	CD	GLU	A	1798	76.904	13.219	71.758	1.00	16.91
2632	OE1	GLU	A	1798	77.671	12.740	70.878	1.00	22.34
2633	OE2	GLU	A	1798	75.703	12.927	71.844	1.00	21.23
2634	C	GLU	A	1798	77.146	17.964	73.246	1.00	9.11
2635	O	GLU	A	1798	76.169	18.329	73.887	1.00	8.72
2636	N	TYR	A	18079	77.735	18.722	72.346	1.00	7.73
2638	CA	TYR	A	18079	77.237	20.070	72.126	1.00	7.44
2640	CB	TYR	A	18079	78.063	21.093	72.962	1.00	8.20
2643	CG	TYR	A	18079	79.505	21.210	72.494	1.00	7.70
2644	CD1	TYR	A	18079	79.860	22.025	71.428	1.00	9.52
2646	CE1	TYR	A	18079	81.122	22.075	70.956	1.00	10.78
2648	CZ	TYR	A	18079	82.122	21.322	71.563	1.00	11.33
2649	OH	TYR	A	18079	83.392	21.365	71.077	1.00	12.64
2651	CE2	TYR	A	18079	81.805	20.521	72.633	1.00	9.69
2653	CD2	TYR	A	18079	80.513	20.464	73.085	1.00	9.33
2655	C	TYR	A	18079	77.302	20.456	70.658	1.00	7.90
2656	O	TYR	A	18079	78.018	19.847	69.861	1.00	7.13
2657	N	TRP	A	1810	76.552	21.511	70.358	1.00	7.24
2659	CA	TRP	A	1810	76.637	22.256	69.143	1.00	7.16
2661	CB	TRP	A	1810	75.238	22.605	68.635	1.00	7.34
2664	CG	TRP	A	1810	74.408	21.443	68.228	1.00	6.74
2665	CD1	TRP	A	1810	73.331	20.944	68.863	1.00	7.18
2667	NE1	TRP	A	1810	72.831	19.856	68.177	1.00	7.84
2669	CE2	TRP	A	1810	73.612	19.657	67.073	1.00	7.15
2670	CD2	TRP	A	1810	74.605	20.643	67.063	1.00	7.46
2671	CE3	TRP	A	1810	75.554	20.640	66.041	1.00	7.76
2673	CZ3	TRP	A	1810	75.472	19.667	65.052	1.00	8.31

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2675	CH2	TRP	A	1810	74.457	18.711	65.088	1.00	8.20
2677	CZ2	TRP	A	1810	73.518	18.689	66.058	1.00	7.45
2679	C	TRP	A	1810	77.351	23.555	69.471	1.00	7.52
2680	O	TRP	A	1810	77.039	24.199	70.469	1.00	8.73
2681	N	LEU	A	1821	78.289	23.952	68.638	1.00	7.47
2683	CA	LEU	A	1821	78.993	25.205	68.849	1.00	8.17
2685	CB	LEU	A	1821	80.425	25.114	68.377	1.00	9.09
2688	CG	LEU	A	1821	81.276	26.367	68.553	1.00	10.77
2690	CD1	LEU	A	1821	81.449	26.692	70.017	1.00	12.41
2694	CD2	LEU	A	1821	82.633	26.143	67.904	1.00	13.16
2698	C	LEU	A	1821	78.249	26.265	68.068	1.00	8.25
2699	O	LEU	A	1821	78.206	26.205	66.829	1.00	8.17
2700	N	VAL	A	1832	77.678	27.240	68.765	1.00	7.63
2702	CA	VAL	A	1832	76.808	28.220	68.146	1.00	7.97
2704	CB	VAL	A	1832	75.454	28.167	68.810	1.00	8.74
2706	CG1	VAL	A	1832	74.544	29.283	68.332	1.00	9.15
2710	CG2	VAL	A	1832	74.817	26.809	68.590	1.00	9.78
2714	C	VAL	A	1832	77.377	29.628	68.256	1.00	8.32
2715	O	VAL	A	1832	77.752	30.084	69.352	1.00	8.39
2716	N	LYS	A	1843	77.480	30.293	67.122	1.00	7.51
2718	CA	LYS	A	1843	77.860	31.689	67.039	1.00	7.53
2720	CB	LYS	A	1843	78.501	31.952	65.693	1.00	7.37
2723	CG	LYS	A	1843	79.094	33.330	65.554	1.00	7.75
2726	CD	LYS	A	1843	79.435	33.681	64.102	1.00	9.08
2729	CE	LYS	A	1843	80.356	34.918	63.980	1.00	10.20
2732	NZ	LYS	A	1843	80.428	35.449	62.603	1.00	10.58
2736	C	LYS	A	1843	76.635	32.535	67.168	1.00	7.84
2737	O	LYS	A	1843	75.696	32.403	66.390	1.00	7.03
2738	N	ASN	A	1854	76.600	33.384	68.182	1.00	7.72
2740	CA	ASN	A	1854	75.489	34.287	68.394	1.00	8.40
2742	CB	ASN	A	1854	75.172	34.300	69.892	1.00	8.73
2745	CG	ASN	A	1854	73.834	34.928	70.241	1.00	8.85
2746	OD1	ASN	A	1854	73.010	35.241	69.374	1.00	10.62
2747	ND2	ASN	A	1854	73.624	35.155	71.537	1.00	10.62
2750	C	ASN	A	1854	75.862	35.664	67.831	1.00	8.86
2751	O	ASN	A	1854	76.995	35.865	67.386	1.00	9.97
2752	N	SER	A	1865	74.924	36.608	67.856	1.00	8.64
2754	CA	SER	A	1865	75.125	37.954	67.352	1.00	8.52
2756	CB	SER	A	1865	74.254	38.212	66.119	1.00	8.51
2759	OG	SER	A	1865	72.928	37.811	66.345	1.00	10.18
2761	C	SER	A	1865	74.824	38.989	68.442	1.00	8.57
2762	O	SER	A	1865	74.280	40.047	68.168	1.00	9.56
2763	N	TRP	A	1876	75.241	38.687	69.666	1.00	8.49
2765	CA	TRP	A	1876	75.092	39.629	70.783	1.00	8.55
2767	CB	TRP	A	1876	74.364	39.005	71.963	1.00	8.15
2770	CG	TRP	A	1876	72.936	38.670	71.670	1.00	9.02
2771	CD1	TRP	A	1876	72.212	39.018	70.563	1.00	9.90
2773	NE1	TRP	A	1876	70.939	38.506	70.654	1.00	11.51
2775	CE2	TRP	A	1876	70.833	37.779	71.808	1.00	10.30
2776	CD2	TRP	A	1876	72.073	37.866	72.477	1.00	9.40
2777	CE3	TRP	A	1876	72.223	37.205	73.696	1.00	11.10

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2779	CZ3	TRP	A	1876	71.146	36.500	74.214	1.00	11.94
2781	CH2	TRP	A	1876	69.938	36.435	73.520	1.00	12.36
2783	CZ2	TRP	A	1876	69.763	37.068	72.324	1.00	12.04
2785	C	TRP	A	1876	76.462	40.131	71.244	1.00	9.10
2786	O	TRP	A	1876	76.651	40.493	72.414	1.00	9.20
2787	N	GLY	A	1887	77.413	40.172	70.328	1.00	8.87
2789	CA	GLY	A	1887	78.747	40.633	70.656	1.00	9.53
2792	C	GLY	A	1887	79.559	39.649	71.462	1.00	10.86
2793	O	GLY	A	1887	79.114	38.578	71.837	1.00	10.90
2794	N	HIS	A	1898	80.785	40.048	71.763	1.00	12.56
2796	CA	HIS	A	1898	81.678	39.190	72.538	1.00	15.23
2798	CB	HIS	A	1898	83.106	39.673	72.405	1.00	16.17
2801	CG	HIS	A	1898	·83.577	39.734	70.999	1.00	19.95
2802	ND1	HIS	A	1898	84.158	38.663	70.359	1.00	26.55
2804	CE1	HIS	A	1898	84.473	39.016	69.125	1.00	26.49
2806	NE2	HIS	A	1898	84.100	40.270	68.939	1.00	27.65
2808	CD2	HIS	A	1898	83.547	40.746	70.102	1.00	24.11
2810	C	HIS	A	1898	81.373	39.062	74.011	1.00	14.64
2811	O	HIS	A	1898	81.915	38.156	74.642	1.00	15.50
2812	N	ASN	A	19089	80.511	39.916	74.574	1.00	14.92
2814	CA	ASN	A	19089	80.164	39.837	76.006	1.00	15.35
2816	CB	ASN	A	189—90	79.385	41.074	76.470	1.00	16.10
2819	CG	ASN	A	19089	79.148	41.078	77.976	1.00	17.48
2820	OD1	ASN	A	19089	80.053	41.413	78.716	1.00	20.32
2821	ND2	ASN	A	19089	77.959	40.651	78.435	1.00	17.49
2824	C	ASN	A	19089	79.320	38.623	76.315	1.00	14.68
2825	O	ASN	A	19089	79.258	38.127	˙77.446	1.00	16.24
2826	N	PHE	A	1910	78.651	38.152	75.289	1.00	12.73
2828	CA	PHE	A	1910	77.776	37.038	75.473	1.00	11.79
2830	CB	PHE	A	1910	76.765	36.983	74.348	1.00	11.21
2833	CG	PHE	A	1910	75.981	35.719	74.356	1.00	11.11
2834	CD1	PHE	A	1910	76.327	34.679	73.526	1.00	11.28
2836	CE1	PHE	A	1910	75.630	33.484	73.579	1.00	10.09
2838	CZ	PHE	A	1910	74.591	33.347	74.463	1.00	13.66
2840	CE2	PHE	A	1910	74.253	34.371	75.285	1.00	12.49
2842	CD2	PHE	A	1910	74.946	35.533	75.256	1.00	12.71
2844	C	PHE	A	1910	78.538	35.709	75.505	1.00	11.39
2845	O	PHE	A	1910	79.409	35.476	74.662	1.00	10.84
2846	N	GLY	A	1921	78.151	34.854	76.458	1.00	12.40
2848	CA	GLY	A	1921	78.728	33.532	76.624	1.00	12.52
2851	C	GLY	A	1921	80.248	33.471	76.564	1.00	13.04
2852	O	GLY	A	1921	80.917	34.201	77.307	1.00	13.76
2853	N	ALA	A	1922	80.771	32.661	75.631	1.00	11.69
2855	CA	ALA	A	1932	82.193	32.403	75.468	˙1.00	12.15
2857	CB	ALA	A	1932	˙82.484	30.929	75.319	1.00	13.90
2861	C	ALA	A	1932	82.678	33.182	74.239	1.00	12.26
2862	O	ALA	A	1932	82.768	32.656	73.133	1.00	10.86
2863	N	GLU	A	1943	82.949	34.461	74.444	1.00	12.26
2865	CA	GLU	A	1943	83.389	35.354	73.385	1.00	12.28
2867	CB	GLU	A	1943	84.776	35.017	72.912	1.00	13.78
2870	CG	GLU	A	1943	85.798	35.053	74.048	1.00	15.01

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2873	CD	GLU	A	1943	86.099	36.436	74.612	1.00	19.69
2874	OE1	GLU	A	1943	85.781	37.478	73.964	1.00	19.31
2875	OE2	GLU	A	1943	86.730	36.480	75.702	1.00	22.60
2876	C	GLU	A	1943	82.419	35.387	72.208	1.00	10.40
2877	O	GLU	A	1943	82.829	35.504	71.054	1.00	10.53
2878	N	GLY	A	1954	81.143	35.300	72.529	1.00	9.77
2880	CA	GLY	A	1954	80.109	35.433	71.531	1.00	8.91
2883	C	GLY	A	1954	79.483	34.119	71.133	1.00	8.59
2884	O	GLY	A	1954	78.509	34.109	70.380	1.00	9.00
2885	N	TYR	A	1965	80.028	33.024	71.650	1.00	8.38
2887	CA	TYR	A	1965	79.592	31.674	71.339	1.00	8.53
2889	CB	TYR	A	1965	80.795	30.824	70.913	1.00	7.89
2892	CG	TYR	A	1965	81.383	31.261	69.602	1.00	8.55
2893	CD1	TYR	A	1965	82.238	32.338	69.524	1.00	8.81
2895	CE1	TYR	A	1965	82.746	32.756	68.324	1.00	10.70
2897	CZ	TYR	A	1965	82.368	32.118	67.179	1.00	11.91
2898	OH	TYR	A	1965	82.858	32.540	65.961	1.00	14.42
2900	CE2	TYR	A	1965	81.513	31.053	67.227	1.00	11.42
2902	CD2	TYR	A	1965	81.016	30.626	68.421	1.00	10.79
2904	C	TYR	A	1965	78.923	30.999	72.509	1.00	8.55
2905	O	TYR	A	1965	79.186	31.291	73.678	1.00	8.88
2906	N	ILE	A	1976	78.061	30.050	72.196	1.00	7.00
2908	CA	ILE	A	1976	77.416	29.234	73.196	1.00	7.38
2910	CB	ILE	A	1976	75.957	29.684	73.506	1.00	8.02
2912	CG1	ILE	A	1976	75.283	28.738	74.508	1.00	8.29
2915	CD1	ILE	A	1976	74.007	29.325	75.074	1.00	8.75
2919	CG2	ILE	A	1976	75.101	29.818	72.269	1.00	8.39
2923	C	ILE	A	1976	77.509	27.780	72.736	1.00	8.49
2924	O	ILE	A	1976	77.294	27.461	71.578	1.00	8.35
2925	N	ARG	A	1987	77.723	26.883	73.665	1.00	8.54
2927	CA	ARG	A	1987	77.814	25.466	73.377	1.00	8.93
2929	CB	ARG	A	1987	78.945	24.754	74.122	1.00	8.40
2932	CG	ARG	A	1987	80.296	25.233	73.751	1.00	12.01
2935	CD	ARG	A	1987	81.362	24.260	74.180	1.00	16.18
2938	NE	ARG	A	1987	82.589	24.922	74.592	1.00	20.61
2940	CZ	ARG	A	1987	83.662	24.267	74.984	1.00	28.20
2941	NH1	ARG	A	1987	83.678	22.935	75.011	1.00	31.60
2944	NH2	ARG	A	1987	84.736	24.945	75.340	1.00	30.70
2947	C	ARG	A	1987	76.465	24.990	73.863	1.00	8.74
2948	O	ARG	A	1987	76.145	25.140	75.044	1.00	9.35
2949	N	MET	A	1998	75.626	24.488	72.955	1.00	9.08
2951	CA	MET	A	1998	74.280	24.075	73.275	1.00	8.70
2953	CB	MET	A	1998	73.305	24.743	72.288	1.00	9.67
2956	CG	MET	A	1998	73.354	26.254	72.393	1.00	10.15
2959	SD	MET	A	1998	72.108	27.123	71.394	1.00	12.72
2960	CE	MET	A	1998	70.651	26.623	72.280	1.00	13.68
2964	C	MET	A	1998	74.147	22.550	73.224	1.00	8.33
2965	O	MET	A	1998	74.754	21.916	72.374	1.00	9.38
2966	N	ALA	A	200199	73.345	21.982	74.109	1.00	8.62
2968	CA	ALA	A	200199	73.202	20.518	74.212	1.00	8.61
2970	CB	ALA	A	200199	72.196	20.147	75.247	1.00	9.19

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
2974	C	ALA	A	200~~199~~	72.826	19.882	72.879	1.00	8.85
2975	O	ALA	A	200~~199~~	71.914	20.335	72.189	1.00	9.50
2976	N	ARG	A	201~~0~~	73.566	18.837	72.537	1.00	8.05
2978	CA	ARG	A	201~~0~~	73.376	18.105	71.288	1.00	8.44
2980	CB	ARG	A	201~~0~~	74.659	18.103	70.505	1.00	8.65
2983	CG	ARG	A	201~~0~~	74.695	17.217	69.263	1.00	8.03
2986	CD	ARG	A	201~~0~~	75.860	17.552	68.385	1.00	8.05
2989	NE	ARG	A	201~~0~~	77.141	17.144	68.974	1.00	8.96
2991	CZ	ARG	A	201~~0~~	77.710	15.974	68.739	1.00	10.43
2992	NH1	ARG	A	201~~0~~	77.119	15.094	67.921	1.00	11.68
2995	NH2	ARG	A	201~~0~~	78.862	15.663	69.317	1.00	11.45
2998	C	ARG	A	201~~0~~	72.936	16.690	71.601	1.00	9.25
2999	O	ARG	A	201~~0~~	73.381	16.085	72.588	1.00	10.70
3000	N	ASN	A	202~~1~~	72.068	16.161	70.751	1.00	10.22
3002	CA	ASN	A	202~~1~~	71.475	14.832	70.919	1.00	12.06
3004	CB	ASN	A	202~~1~~	72.508	13.737	70.742	1.00	12.00
3007	CG	ASN	A	202~~1~~	73.074	13.694	69.349	1.00	13.75
3008	OD1	ASN	A	202~~1~~	72.403	14.051	68.379	1.00	19.63
3009	ND2	ASN	A	202~~1~~	74.326	13.292	69.232	1.00	16.84
3012	C	ASN	A	202~~1~~	70.723	14.694	72.244	1.00	12.14
3013	O	ASN	A	202~~1~~	70.695	13.627	72.866	1.00	13.57
3014	N	LYS	A	203~~2~~	70.100	15.784	72.674	1.00	12.78
3016	CA	LYS	A	203~~2~~	69.270	15.821	73.840	1.00	12.82
3018	CB	LYS	A	203~~2~~	69.814	16.817	74.858	1.00	13.07
3021	CG	LYS	A	203~~2~~	71.099	16.359	75.488	1.00	15.16
3024	CD	LYS	A	203~~2~~	70.895	15.148	76.335	1.00	17.36
3027	CE	LYS	A	203~~2~~	72.119	14.878	77.168	1.00	20.65
3030	NZ	LYS	A	203~~2~~	72.037	13.539	77.804	1.00	24.01
3034	C	LYS	A	203~~2~~	67.849	16.216	73.404	1.00	12.76
3035	O	LYS	A	203~~2~~	67.257	17.163	73.930	1.00	13.51
3036	N	GLY	A	204~~3~~	67.322	15.491	72.424	1.00	13.21
3038	CA	GLY	A	204~~3~~	65.961	15.713	71.985	1.00	12.63
3041	C	GLY	A	204~~3~~	65.728	17.037	71.270	1.00	11.61
3042	O	GLY	A	204~~3~~	64.692	17.672	71.498	1.00	12.80
3043	N	ASN	A	205~~4~~	66.647	17.429	70.400	1.00	10.39
3045	CA	ASN	A	205~~4~~	66.486	18.663	69.638	1.00	10.31
3047	CB	ASN	A	205~~4~~	65.294	18.601	68.694	1.00	10.00
3050	CG	ASN	A	205~~4~~	65.225	19.805	67.791	1.00	9.81
3051	OD1	ASN	A	205~~4~~	66.220	20.472	67.595	1.00	11.31
3052	ND2	ASN	A	205~~4~~	64.054	20.083	67.241	1.00	9.87
3055	C	ASN	A	205~~4~~	66.297	19.815	70.630	1.00	9.86
3056	O	ASN	A	205~~4~~	65.355	20.603	70.580	1.00	9.58
3057	N	HIS	A	206~~5~~	67.243	19.900	71.538	1.00	9.50
3059	CA	HIS	A	206~~5~~	67.184	20.879	72.602	1.00	9.83
3061	CB	HIS	A	206~~5~~	68.366	20.685	73.541	1.00	10.75
3064	CG	HIS	A	206~~5~~	68.193	21.365	74.855	1.00	12.73
3065	ND1	HIS	A	206~~5~~	69.046	22.351	75.288	1.00	18.83
3067	CE1	HIS	A	206~~5~~	68.673	22.748	76.491	1.00	13.41
3069	NE2	HIS	A	206~~5~~	67.578	22.093	76.830	1.00	18.21
3071	CD2	HIS	A	206~~5~~	67.284	21.178	75.842	1.00	16.24
3073	C	HIS	A	206~~5~~	67.151	22.312	72.059	1.00	9.05

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3074	O	HIS	A	2065	67.970	22.705	71.217	1.00	9.40
3075	N	CYS	A	2076	66.181	23.068	72.564	1.00	9.67
3077	CA	CYS	A	2076	65.987	24.462	72.183	1.00	10.09
3079	CB	CYS	A	2076	67.213	25.301	72.537	1.00	11.22
3082	SG	CYS	A	2076	67.454	25.464	74.328	1.00	14.76
3083	C	CYS	A	2076	65.668	24.601	70.710	1.00	8.96
3084	O	CYS	A	2076	65.742	25.695	70.181	1.00	9.52
3085	N	GLY	A	2087	65.254	23.507	70.074	1.00	8.20
3087	CA	GLY	A	2087	64.903	23.559	68.666	1.00	7.73
3090	C	GLY	A	2087	66.068	23.774	67.706	1.00	7.74
3091	O	GLY	A	2087	65.874	24.175	66.557	1.00	8.40
3092	N	ILE	A	2098	67.290	23.502	68.157	1.00	8.32
3094	CA	ILE	A	2098	68.458	23.775	67.344	1.00	8.73
3096	CB	ILE	A	2098	69.739	23.411	68.128	1.00	9.51
3098	CG1	ILE	A	2098	70.946	23.964	67.392	1.00	13.12
3101	CD1	ILE	A	2098	72.002	24.462	68.282	1.00	14.36
3105	CG2	ILE	A	2098	69.825	21.946	68.410	1.00	11.21
3109	C	ILE	A	2098	68.412	23.134	65.963	1.00	8.50
3110	O	ILE	A	2098	68.844	23.767	64.984	1.00	8.73
3111	N	ALA	A	21009	67.845	21.934	65.866	1.00	8.43
3113	CA	ALA	A	21009	67.805	21.244	64.584	1.00	8.37
3115	CB	ALA	A	21009	68.177	19.781	64.754	1.00	8.70
3119	C	ALA	A	21009	66.451	21.360	63.933	1.00	8.52
3120	O	ALA	A	21009	66.175	20.669	62.961	1.00	9.00
3121	N	SER	A	2110	65.603	22.227	64.454	1.00	8.50
3123	CA	SER	A	2110	64.267	22.387	63.897	1.00	8.56
3125	CB	SER	A	2110	63.423	23.278	64.785	1.00	9.59
3128	OG	SER	A	2110	63.135	22.632	65.999	1.00	8.77
3130	C	SER	A	2110	64.272	22.931	62.469	1.00	9.47
3131	O	SER	A	2110	63.656	22.333	61.579	1.00	9.57
3132	N	PHE	A	2121	64.958	24.054	62.252	1.00	8.64
3134	CA	PHE	A	2121	64.942	24.725	60.946	1.00	8.51
3136	CB	PHE	A	2121	64.040	25.940	61.020	1.00	9.02
3139	CG	PHE	A	2121	62.609	25.603	61.358	1.00	10.68
3140	CD1	PHE	A	2121	62.108	25.848	62.629	1.00	11.62
3142	CE1	PHE	A	2121	60.808	25.513	62.953	1.00	13.92
3144	CZ	PHE	A	2121	60.002	24.940	62.020	1.00	13.43
3146	CE2	PHE	A	2121	60.482	24.668	60.757	1.00	13.66
3148	CD2	PHE	A	2121	61.794	24.990	60.425	1.00	13.75
3150	C	PHE	A	2121	66.341	25.109	60.449	1.00	7.85
3151	O	PHE	A	2121	66.668	26.297	60.359	1.00	7.35
3152	N	PRO	A	2132	67.171	24.132	60.137	1.00	7.87
3153	CA	PRO	A	2132	68.526	24.411	59.657	1.00	7.91
3155	CB	PRO	A	2132	69.280	23.118	59.944	1.00	8.05
3158	CG	PRO	A	2132	68.326	22.271	60.751	1.00	9.03
3161	CD	PRO	A	2132	66.970	22.685	60.324	1.00	8.17
3164	C	PRO	A	2132	68.569	24.645	58.168	1.00	7.81
3165	O	PRO	A	2132	67.835	24.004	57.417	1.00	8.66
3166	N	SER	A	2143	69.451	25.511	57.731	1.00	7.67
3168	CA	SER	A	2143	69.589	25.767	56.316	1.00	8.91
3170	CB	SER	A	2143	68.585	26.823	55.843	1.00	9.92

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3173	OG	SER	A	2143	68.686	28.029	56.549	1.00	9.41
3175	C	SER	A	2143	70.990	26.242	56.018	1.00	8.74
3176	O	SER	A	2143	71.644	26.890	56.854	1.00	8.41
3177	N	TYR	A	2144	71.488	25.965	54.820	1.00	8.11
3179	CA	TYR	A	2154	72.770	26.496	54.419	1.00	8.57
3181	CB	TYR	A	2154	73.878	25.524	54.750	1.00	8.86
3184	CG	TYR	A	2154	73.802	24.225	53.997	1.00	9.58
3185	CD1	TYR	A	2154	73.083	23.162	54.493	1.00	10.93
3187	CE1	TYR	A	2154	73.014	21.984	53.824	1.00	12.85
3189	CZ	TYR	A	2154	73.660	21.840	52.629	1.00	14.08
3190	OH	TYR	A	2154	73.595	20.638	51.932	1.00	17.38
3192	CE2	TYR	A	2154	74.387	22.870	52.098	1.00	13.57
3194	CD2	TYR	A	2154	74.460	24.066	52.792	1.00	11.80
3196	C	TYR	A	2154	72.771	26.825	52.939	1.00	8.35
3197	O	TYR	A	2154	72.071	26.171	52.148	1.00	8.32
3198	N	PRO	A	2165	73.505	27.849	52.554	1.00	8.33
3199	CA	PRO	A	2165	73.558	28.279	51.164	1.00	9.32
3201	CB	PRO	A	2165	.73.838	29.766	51.292	1.00	9.52
3204	CG	PRO	A	2165	74.640	29.869	52.609	1.00	9.40
3207	CD	PRO	A	2165	74.338	28.694	53.428	1.00	9.08
3210	C	PRO	A	2165	74.715	27.668	50.448	1.00	10.44
3211	O	PRO	A	2165	75.616	27.154	51.078	1.00	10.23
3212	N	GLU	A	2176	74.693	27.738	49.130	1.00	11.74
3214	CA	GLU	A	2176	75.860	27.352	48.371	1.00	14.22
3216	CB	GLU	A	2176	75.713	25.946	47.826	1.00	15.79
3219	CG	GLU	A	2176	75.928	24.888	48.913	1.00	19.53
3222	CD	GLU	A	2176	75.598	23.485	48.437	1.00	23.19
3223	OE1	GLU	A	2176	76.533	22.762	48.014	1.00	28.75
3224	OE2	GLU	A	2176	74.412	23.116	48.460	1.00	20.95
3225	C	GLU	A	2176	76.147	28.401	47.307	1.00	15.13
3226	O	GLU	A	2176	75.261	29.132	46.859	1.00	14.99
3227	N	ILE	A	2187	77.421	28.537	46.971	1.00	16.50
3229	CA	ILE	A	2187	77.837	29.462	45.940	1.00	18.88
3231	CB	ILE	A	2187	79.033	30.267	46.443	1.00	18.61
3233	CG1	ILE	A	2187	78.692	30.969	47.755	1.00	18.17
3236	CD1	ILE	A	2187	79.837	31.846	48.272	1.00	18.40
3240	CG2	ILE	A	2187	79.446	31.297	45.400	1.00	18.53
3244	C	ILE	A	2187	78.212	28.569	44.771	1.00	22.02
3245	O	ILE	A	2187	79.245	27.903	44.798	1.00	22.95
3246	N	GLY	A	2198	77.323	28.493	43.793	1.00	25.34
3248	CA	GLY	A	2198	77.477	27.585	42.661	1.00	26.67
3251	C	GLY	A	2198	78.770	26.797	42.691	1.00	28.29
3252	O	GLY	A	2198	79.804	27.285	42.206	1.00	30.46
3253	O5	E64	A	22019	60.443	35.689	64.169	1.00	23.18
3254	C11	E64	A	22019	61.269	35.440	63.307	1.00	23.53
3255	C6	E64	A	22019	62.709	35.061	63.604	1.00	19.61
3257	C7	E64	A	22019	62.844	33.610	64.019	1.00	18.27
3260	C8	E64	A	22019	64.294	33.135	64.052	1.00	17.47
3262	C10	E64	A	22019	65.114	33.414	62.804	1.00	17.99
3266	C9	E64	A	22019	64.309	31.638	64.321	1.00	19.43
3270	N1	E64	A	22019	63.254	35.884	64.676	1.00	19.19

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3272	C4	E64	A	220~~19~~	63.918	37.003	64.371	1.00	21.88
3273	O4	E64	A	220~~19~~	64.113	37.313	63.228	1.00	20.92
3274	C3	E64	A	220~~19~~	64.450	37.903	65.449	1.00	24.96
3276	O3	E64	A	220~~19~~	63.338	38.352	66.185	1.00	27.29
3278	C2	E64	A	220~~19~~	65.405	37.161	66.372	1.00	25.08
3281	C1	E64	A	220~~19~~	66.483	38.064	66.930	1.00	26.84
3282	O2	E64	A	220~~19~~	67.021	39.002	66.164	1.00	23.76
3284	O1	E64	A	220~~19~~	66.875	37.917	68.078	1.00	25.07
3285	N2	E64	A	220~~19~~	61.155	35.463	61.989	1.00	24.93
3287	C12	E64	A	220~~19~~	60.197	35.736	60.942	1.00	29.49
3290	C13	E64	A	220~~19~~	59.154	36.783	61.210	1.00	30.80
3293	C14	E64	A	220~~19~~	58.960	37.407	59.826	1.00	32.35
3296	C15	E64	A	220~~19~~	58.183	38.708	59.769	1.00	32.03
3299	N3	E64	A	220~~19~~	57.963	39.165	61.131	1.00	33.36
3301	C16	E64	A	220~~19~~	57.363	40.299	61.469	1.00	35.00
3302	N5	E64	A	220~~19~~	57.230	40.550	62.774	1.00	34.56
3305	N4	E64	A	220~~19~~	56.920	41.164	60.539	1.00	35.50
3308	N	ILE	B	~~0~~ 1	26.179	20.401	122.831	1.00	26.31
3310	CA	ILE	B	1~~0~~	27.481	21.012	123.235	1.00	25.06
3312	CB	ILE	B	1~~0~~	27.757	20.715	124.726	1.00	25.63
3314	CG1	ILE	B	1~~0~~	26.717	21.473	125.571	1.00	26.29
3317	CD1	ILE	B	1~~0~~	26.963	22.985	125.666	1.00	27.69
3321	CG2	ILE	B	1~~0~~	29.144	21.147	125.125	1.00	26.52
3325	C	ILE	B	1~~0~~	28.566	20.528	122.257	1.00	23.29
3326	O	ILE	B	1~~0~~	28.642	19.347	121.941	1.00	25.95
3330	N	LEU	B	2~~1~~	29.283	21.468	121.656	1.00	19.32
3332	CA	LEU	B	2~~1~~	30.356	21.120	120.729	1.00	16.44
3334	CB	LEU	B	2~~1~~	30.248	22.003	119.482	1.00	15.52
3337	CG	LEU	B	2~~1~~	28.925	21.937	118.742	1.00	15.20
3339	CD1	LEU	B	2~~1~~	28.911	22.961	117.652	1.00	16.04
3343	CD2	LEU	B	2~~1~~	28.681	20.533	118.197	1.00	16.50
3347	C	LEU	B	2~~1~~	31.715	21.354	121.326	1.00	14.20
3348	O	LEU	B	2~~1~~	31.887	22.219	122.182	1.00	13.39
3349	N	PRO	B	3~~2~~	32.720	20.634	120.831	1.00	12.67
3350	CA	PRO	B	3~~2~~	34.078	20.898	121.290	1.00	12.15
3352	CB	PRO	B	3~~2~~	34.922	19.890	120.508	1.00	12.81
3355	CG	PRO	B	3~~2~~	33.997	18.845	120.014	1.00	15.27
3358	CD	PRO	B	3~~2~~	32.656	19.543	119.849	1.00	13.10
3361	C	PRO	B	3~~2~~	34.521	22.320	120.970	1.00	11.96
3362	O	PRO	B	3~~2~~	34.115	22.902	119.956	1.00	11.24
3363	N	ASP	B	4~~3~~	35.380	22.881	121.804	1.00	11.67
3365	CA	ASP	B	4~~3~~	35.906	24.204	121.564	1.00	12.03
3367	CB	ASP	B	4~~3~~	36.663	24.692	122.793	1.00	12.55
3370	CG	ASP	B	4~~3~~	35.754	25.094	123.902	1.00	16.27
3371	OD1	ASP	B	4~~3~~	34.550	25.364	123.641	1.00	17.55
3372	OD2	ASP	B	4~~3~~	36.175	25.179	125.072	1.00	19.92
3373	C	ASP	B	4~~3~~	36.844	24.267	120.350	1.00	11.11
3374	O	ASP	B	4~~3~~	36.999	25.309	119.726	1.00	11.94
3375	N	SER	B	~~4~~ 5	37.503	23.159	120.069	1.00	10.88
3377	CA	SER	B	~~4~~ 5	38.422	23.056	118.956	1.00	10.69
3379	CB	SER	B	~~4~~ 5	39.862	23.278	119.379	1.00	12.28

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3382	OG	SER	B	4 5	40.030	24.483	120.073	1.00	13.59
3384	C	SER	B	4 5	38.326	21.671	118.351	1.00	10.39
3385	O	SER	B	4 5	38.131	20.682	119.048	1.00	10.09
3386	N	VAL	B	5 6	38.490	21.608	117.042	1.00	9.75
3388	CA	VAL	B	5 6	38.504	20.335	116.339	1.00	10.30
3390	CB	VAL	B	5 6	37.162	20.018	115.648	1.00	11.95
3392	CG1	VAL	B	65	37.172	18.668	114.950	1.00	14.73
3396	CG2	VAL	B	65	36.039	19.995	116.635	1.00	11.35
3400	C	VAL	B	65	39.609	20.393	115.293	1.00	9.19
3401	O	VAL	B	65	39.846	21.447	114.715	1.00	8.51
3402	N	ASP	B	76	40.291	19.276	115.069	1.00	9.75
3404	CA	ASP	B	76	41.268	19.192	113.994	1.00	9.60
3406	CB	ASP	B	76	42.695	19.447	114.522	1.00	9.52
3409	CG	ASP	B	76	43.746	19.537	113.411	1.00	10.94
3410	OD1	ASP	B	76	43.502	19.061	112.278	1.00	11.14
3411	OD2	ASP	B	76	44.860	20.105	113.604	1.00	13.70
3412	C	ASP	B	76	41.201	17.790	113.401	1.00	9.72
3413	O	ASP	B	76	41.672	16.814	114.013	1.00	10.06
3414	N	TRP	B	87	40.619	17.660	112.212	1.00	8.47
3416	CA	TRP	B	7 8	40.422	16.343	111.617	1.00	8.47
3418	CB	TRP	B	87	39.438	16.421	110.438	1.00	8.76
3421	CG	TRP	B	87	38.010	16.550	110.910	1.00	9.31
3422	CD1	TRP	B	87	37.268	17.706	111.021	1.00	8.05
3424	NE1	TRP	B	87	36.022	17.417	111.530	1.00	9.00
3426	CE2	TRP	B	87	35.943	16.076	111.776	1.00	13.39
3427	CD2	TRP	B	87	37.173	15.499	111.400	1.00	14.09
3428	CE3	TRP	B	87	37.348	14.123	111.590	1.00	18.93
3430	CZ3	TRP	B	87	36.306	13.389	112.125	1.00	21.96
3432	CH2	TRP	B	87	35.091	13.992	112.462	1.00	19.55
3434	CZ2	TRP	B	87	34.888	15.325	112.297	1.00	16.30
3436	C	TRP	B	87	41.715	15.667	111.212	1.00	8.59
3437	O	TRP	B	87	41.734	14.483	110.905	1.00	9.41
3438	N	ARG	B	98	42.798	16.418	111.194	1.00	8.31
3440	CA	ARG	B	98	44.066	15.806	110.879	1.00	9.20
3442	CB	ARG	B	98	45.133	16.865	110.690	1.00	8.81
3445	CG	ARG	B	98	44.866	17.793	109.504	1.00	9.65
3448	CD	ARG	B	98	45.809	18.931	109.353	1.00	8.75
3451	NE	ARG	B	98	45.874	19.766	110.535	1.00	8.53
3453	CZ	ARG	B	98	46.726	20.763	110.692	1.00	10.89
3454	NH1	ARG	B	98	47.558	21.110	109.709	1.00	9.82
3457	NH2	ARG	B	98	46.745	21.416	111.831	1.00	9.81
3460	C	ARG	B	98	44.457	14.843	111.991	1.00	9.40
3461	O	ARG	B	98	45.120	13.834	111.744	1.00	9.91
3462	N	GLU	B	109	44.032	15.169	113.206	1.00	10.75
3464	CA	GLU	B	910	44.342	14.390	114.392	1.00	12.72
3466	CB	GLU	B	10 9	43.976	15.159	115.659	1.00	12.86
3469	CG	GLU	B	10 9	44.908	16.267	116.030	1.00	16.15
3472	CD	GLU	B	10 9	44.483	16.965	117.281	1.00	18.62
3473	OE1	GLU	B	10 9	43.648	16.384	118.010	1.00	24.05
3474	OE2	GLU	B	10 9	44.974	18.080	117.521	1.00	21.53
3475	C	GLU	B	10 9	43.614	13.074	114.422	1.00	14.16

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3476	O	GLU	B	10—9	43.905	12.234	115.282	1.00	15.74
3477	N	LYS	B	110	42.609	12.943	113.537	1.00	13.88
3479	CA	LYS	B	110	41.818	11.726	113.382	1.00	15.05
3481	CB	LYS	B	110	40.324	12.048	113.324	1.00	16.00
3484	CG	LYS	B	110	39.480	10.931	113.942	1.00	21.01
3487	CD	LYS	B	110	38.022	11.096	113.640	1.00	24.23
3490	CE	LYS	B	110	37.225	9.847	114.002	1.00	24.82
3493	NZ	LYS	B	110	37.039	9.691	115.470	1.00	27.97
3497	C	LYS	B	110	42.203	10.941	112.127	1.00	14.16
3498	O	LYS	B	110	41.555	9.961	111.764	1.00	15.76
3499	N	GLY	B	121	43.235	11.376	111.420	1.00	12.26
3501	CA	GLY	B	121	43.717	10.637	110.283	1.00	12.43
3504	C	GLY	B	121	42.803	10.716	109.074	1.00	11.52
3505	O	GLY	B	121	42.854	9.844	108.202	1.00	11.94
3506	N	CYS	B	132	42.016	11.791	108.988	1.00	10.65
3508	CA	CYS	B	132	41.020	11.954	107.921	1.00	10.35
3510	CB	CYS	B	132	39.686	12.387	108.538	1.00	10.42
3513	SG	CYS	B	132	38.895	11.060	109.450	1.00	13.71
3514	C	CYS	B	132	41.383	12.965	106.860	1.00	9.86
3515	O	CYS	B	132	40.539	13.297	106.013	1.00	10.30
3516	N	VAL	B	143	42.621	13.432	106.862	1.00	8.32
3518	CA	VAL	B	143	43.035	14.460	105.930	1.00	7.80
3520	CB	VAL	B	143	43.238	15.799	106.644	1.00	7.81
3522	CG1	VAL	B	143	43.589	16.866	105.684	1.00	9.67
3526	CG2	VAL	B	143	42.006	16.211	107.388	1.00	7.81
3530	C	VAL	B	143	44.303	14.021	105.225	1.00	8.11
3531	O	VAL	B	143	45.267	13.632	105.866	1.00	8.74
3532	N	THR	B	154	44.306	14.054	103.901	1.00	8.18
3534	CA	THR	B	154	45.465	13.638	103.154	1.00	8.66
3536	CB	THR	B	154	45.065	13.204	101.736	1.00	8.73
3538	OG1	THR	B	154	44.449	14.317	101.062	1.00	9.54
3540	CG2	THR	B	154	44.049	12.116	101.773	1.00	9.61
3544	C	THR	B	154	46.505	14.757	103.058	1.00	8.98
3545	O	THR	B	154	46.308	15.876	103.544	1.00	9.62
3546	N	GLU	B	165	47.589	14.452	102.374	1.00	10.04
3548	CA	GLU	B	165	48.623	15.430	102.108	1.00	10.66
3550	CB	GLU	B	165	49.744	14.786	101.282	1.00	12.98
3553	CG	GLU	B	165	50.511	13.721	102.016	1.00	18.14
3556	CD	GLU	B	165	49.944	12.321	101.838	1.00	24.98
3557	OE1	GLU	B	165	48.842	12.170	101.225	1.00	28.47
3558	OE2	GLU	B	165	50.597	11.363	102.341	1.00	30.56
3559	C	GLU	B	165	48.060	16.600	101.308	1.00	9.92
3560	O	GLU	B	165	47.102	16.454	100.538	1.00	9.64
3561	N	VAL	B	176	48.621	17.773	101.540	1.00	9.32
3563	CA	VAL	B	176	48.275	18.963	100.791	1.00	9.51
3565	CB	VAL	B	176	48.929	20.226	101.407	1.00	9.68
3567	CG1	VAL	B	176	48.725	21.419	100.515	1.00	10.32
3571	CG2	VAL	B	176	48.346	20.472	102.794	1.00	10.05
3575	C	VAL	B	176	48.715	18.800	99.345	1.00	9.70
3576	O	VAL	B	176	49.822	18.337	99.056	1.00	11.33
3577	N	LYS	B	187	47.812	19.164	98.452	1.00	9.14

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3579	CA	LYS	B	18~~7~~	48.036	19.077	97.019	1.00	9.10
3581	CB	LYS	B	18~~7~~	46.792	18.510	96.317	1.00	9.82
3584	CG	LYS	B	18~~7~~	46.286	17.183	96.899	1.00	9.61
3587	CD	LYS	B	18~~7~~	47.394	16.156	96.995	1.00	10.77
3590	CE	LYS	B	18~~7~~	46.863	14.765	97.356	1.00	10.68
3593	NZ	LYS	B	18~~7~~	45.971	14.681	98.574	1.00	10.54
3597	C	LYS	B	18~~7~~	48.376	20.435	96.444	1.00	9.11
3598	O	LYS	B	18~~7~~	48.175	21.477	97.077	1.00	8.27
3599	N	TYR	B	18~~8~~	48.913	20.392	95.237	1.00	9.99
3601	CA	TYR	B	19~~8~~	49.286	21.576	94.514	1.00	11.00
3603	CB	TYR	B	19~~8~~	50.784	21.553	94.275	1.00	11.58
3606	CG	TYR	B	19~~8~~	51.312	22.759	93.574	1.00	14.54
3607	CD1	TYR	B	19~~8~~	51.731	22.693	92.265	1.00	18.60
3609	CE1	TYR	B	19~~8~~	52.240	23.816	91.622	1.00	19.12
3611	CZ	TYR	B	19~~8~~	52.316	25.009	92.292	1.00	19.72
3612	OH	TYR	B	19~~8~~	52.825	26.133	91.644	1.00	21.52
3614	CE2	TYR	B	19~~8~~	51.898	25.081	93.598	1.00	20.90
3616	CD2	TYR	B	19~~8~~	51.411	23.959	94.227	1.00	16.93
3618	C	TYR	B	19~~8~~	48.530	21.641	93.192	1.00	11.25
3619	O	TYR	B	19~~8~~	48.838	20.875	92.287	1.00	12.20
3620	N	GLN	B	20~~19~~	47.551	22.548	93.085	1.00	10.99
3622	CA	GLN	B	20~~19~~	46.764	22.697	91.854	1.00	11.56
3624	CB	GLN	B	20~~19~~	45.462	23.449	92.128	1.00	11.78
3627	CG	GLN	B	20~~19~~	45.634	24.886	92.479	1.00	11.89
3630	CD	GLN	B	20~~19~~	44.319	25.534	92.805	1.00	14.37
3631	OE1	GLN	B	20~~19~~	43.874	25.500	93.946	1.00	16.74
3632	NE2	GLN	B	20~~19~~	43.682	26.130	91.804	1.00	16.06
3635	C	GLN	B	20~~19~~	47.520	23.342	90.684	1.00	13.08
3636	O	GLN	B	20~~19~~	47.154	23.148	89.532	1.00	13.49
3637	N	GLY	B	21~~0~~	48.538	24.130	90.984	1.00	14.20
3639	CA	GLY	B	21~~0~~	49.291	24.796	89.928	1.00	15.55
3642	C	GLY	B	21~~0~~	48.445	25.838	89.229	1.00	16.58
3643	O	GLY	B	21~~0~~	47.591	26.473	89.824	1.00	17.40
3644	N	SER	B	22~~1~~	48.657	26.014	87.929	1.00	18.41
3646	CA	SER	B	22~~1~~	47.926	27.050	87.216	1.00	19.92
3648	CB	SER	B	22~~1~~	48.786	27.582	86.067	1.00	20.36
3651	OG	SER	B	22~~1~~	49.853	28.330	86.613	1.00	26.52
3653	C	SER	B	22~~1~~	46.571	26.639	86.684	1.00	19.66
3654	O	SER	B	22~~1~~	46.026	27.300	85.804	1.00	22.07
3655	N	CYS	B	23~~2~~	46.014	25.567	87.227	1.00	18.12
3657	CA	CYS	B	23~~2~~	44.734	25.035	86.807	1.00	17.66
3659	CB	CYS	B	23~~2~~	44.859	23.511	86.660	1.00	16.85
3662	SG	CYS	B	23~~2~~	43.329	22.596	86.359	1.00	18.12
3663	C	CYS	B	23~~2~~	43.755	25.406	87.898	1.00	16.72
3664	O	CYS	B	23~~2~~	44.033	25.126	89.059	1.00	17.73
3665	N	GLY	B	24~~3~~	42.641	26.041	87.529	1.00	16.59
3667	CA	GLY	B	24~~3~~	41.629	26.472	88.490	1.00	15.95
3670	C	GLY	B	24~~3~~	40.765	25.313	88.940	1.00	15.26
3671	O	GLY	B	24~~3~~	39.559	25.273	88.674	1.00	17.01
3672	N	ALA	B	25~~4~~	41.415	24.370	89.601	1.00	14.80
3674	CA	ALA	B	25~~4~~	40.766	23.154	90.034	1.00	13.96

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3676	CB	ALA	B	254	41.593	21.949	89.612	1.00	14.69
3680	C	ALA	B	254	40.569	23.131	91.533	1.00	13.78
3681	O	ALA	B	254	40.438	22.075	92.087	1.00	13.20
3682	N	CYS	B	265	40.543	24.295	92.182	1.00	13.59
3684	CA	CYS	B	265	40.310	24.347	93.632	1.00	14.47
3686	CB	CYS	B	265	40.128	25.796	94.108	1.00	15.45
3689	SG	CYS	B	265	38.544	26.600	93.662	1.00	20.16
3690	C	CYS	B	265	39.055	23.578	94.036	1.00	12.35
3691	O	CYS	B	265	39.034	22.876	95.046	1.00	11.94
3692	N	TRP	B	276	38.010	23.741	93.234	1.00	11.67
3694	CA	TRP	B	276	36.712	23.125	93.479	1.00	9.93
3696	CB	TRP	B	276	35.723	23.494	92.368	1.00	10.34
3699	CG	TRP	B	276	36.153	23.127	90.992	1.00	9.14
3700	CD1	TRP	B	276	37.007	23.828	90.172	1.00	12.09
3702	NE1	TRP	B	276	37.140	23.177	88.973	1.00	11.76
3704	CE2	TRP	B	276	36.389	22.035	88.999	1.00	11.13
3705	CD2	TRP	B	276	35.756	21.977	90.258	1.00	10.11
3706	CE3	TRP	B	276	34.888	20.909	90.520	1.00	11.37
3708	CZ3	TRP	B	276	34.704	19.944	89.572	1.00	11.10
3710	CH2	TRP	B	276	35.369	20.015	88.322	1.00	10.07
3712	CZ2	TRP	B	276	36.186	21.072	88.020	1.00	10.00
3714	C	TRP	B	276	36.863	21.608	93.553	1.00	9.89
3715	O	TRP	B	276	36.200	20.960	94.352	1.00	9.28
3716	N	ALA	B	287	37.696	21.067	92.684	1.00	8.71
3718	CA	ALA	B	287	37.884	19.629	92.615	1.00	8.36
3720	CB	ALA	B	287	38.634	19.247	91.352	1.00	8.25
3724	C	ALA	B	287	38.634	19.108	93.827	1.00	8.01
3725	O	ALA	B	287	38.277	18.080	94.381	1.00	9.03
3726	N	PHE	B	298	39.649	19.855	94.247	1.00	8.26
3728	CA	PHE	B	298	40.429	19.478	95.410	1.00	7.81
3730	CB	PHE	B	298	41.688	20.315	95.512	1.00	7.75
3733	CG	PHE	B	298	42.746	19.895	94.552	1.00	9.37
3734	CD1	PHE	B	298	43.018	20.658	93.443	1.00	10.12
3736	CE1	PHE	B	298	43.989	20.270	92.559	1.00	10.86
3738	CZ	PHE	B	298	44.676	19.114	92.761	1.00	10.23
3740	CE2	PHE	B	298	44.409	18.338	93.866	1.00	9.99
3742	CD2	PHE	B	298	43.446	18.735	94.750	1.00	10.89
3744	C	PHE	B	298	39.591	19.605	96.665	1.00	7.26
3745	O	PHE	B	298	39.651	18.759	97.551	1.00	7.71
3746	N	SER	B	3029	38.809	20.666	96.733	1.00	8.11
3748	CA	SER	B	3029	37.921	20.831	97.878	1.00	7.44
3750	CB	SER	B	3029	37.149	22.142	97.725	1.00	8.02
3753	OG	SER	B	3029	36.189	22.268	98.747	1.00	8.99
3755	C	SER	B	3029	36.968	19.650	97.990	1.00	7.35
3756	O	SER	B	3029	36.779	19.077	99.052	1.00	7.73
3757	N	ALA	B	310	36.391	19.273	96.861	1.00	6.79
3759	CA	ALA	B	310	35.434	18.193	96.852	1.00	6.88
3761	CB	ALA	B	310	34.794	18.096	95.474	1.00	6.95
3765	C	ALA	B	310	36.093	16.873	97.239	1.00	7.15
3766	O	ALA	B	310	35.553	16.124	98.065	1.00	7.96
3767	N	VAL	B	321	37.225	16.548	96.634	1.00	7.79

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3769	CA	VAL	B	321	37.829	15.264	96.939	1.00	7.28
3771	CB	VAL	B	321	38.970	14.832	95.997	1.00	8.12
3773	CG1	VAL	B	321	38.462	14.661	94.577	1.00	10.03
3777	CG2	VAL	B	321	40.142	15.765	96.072	1.00	8.65
3781	C	VAL	B	321	38.280	15.247	98.393	1.00	7.08
3782	O	VAL	B	321	38.207	14.198	99.030	1.00	7.98
3783	N	GLY	B	332	38.746	16.377	98.907	1.00	6.99
3785	CA	GLY	B	332	39.178	16.423	100.302	1.00	6.98
3788	C	GLY	B	332	38.043	16.094	101.246	1.00	6.36
3789	O	GLY	B	332	38.182	15.354	102.220	1.00	6.80
3790	N	ALA	B	343	36.864	16.626	100.960	1.00	6.18
3792	CA	ALA	B	343	35.719	16.337	101.795	1.00	6.46
3794	CB	ALA	B	343	34.566	17.200	101.415	1.00	7.31
3798	C	ALA	B	343	35.362	14.861	101.707	1.00	6.99
3799	O	ALA	B	343	35.052	14.220	102.711	1.00	7.66
3800	N	LEU	B	354	35.390	14.309	100.506	1.00	7.18
3802	CA	LEU	B	354	35.040	12.909	100.345	1.00	6.98
3804	CB	LEU	B	354	34.741	12.596	98.869	1.00	6.57
3807	CG	LEU	B	354	34.051	11.242	98.616	1.00	7.96
3809	CD1	LEU	B	354	32.767	11.102	99.367	1.00	9.26
3813	CD2	LEU	B	354	33.818	11.071	97.119	1.00	9.94
3817	C	LEU	B	354	36.088	11.959	100.926	1.00	7.43
3818	O	LEU	B	354	35.732	10.909	101.448	1.00	9.03
3819	N	GLU	B	365	37.354	12.357	100.875	1.00	7.66
3821	CA	GLU	B	365	38.439	11.558	101.420	1.00	8.49
3823	CB	GLU	B	365	39.782	12.285	101.250	1.00	9.64
3826	CG	GLU	B	365	40.304	12.231	99.839	1.00	11.94
3829	CD	GLU	B	365	41.381	13.244	99.509	1.00	12.43
3830	OE1	GLU	B	365	41.796	14.075	100.341	1.00	11.97
3831	OE2	GLU	B	365	41.774	13.223	98.354	1.00	11.89
3832	C	GLU	B	365	38.198	11.303	102.897	1.00	8.34
3833	O	GLU	B	365	38.397	10.201	103.381	1.00	8.33
3834	N	ALA	B	376	37.742	12.325	103.613	1.00	8.11
3836	CA	ALA	B	376	37.459	12.195	105.029	1.00	7.96
3838	CB	ALA	B	376	37.136	13.535	105.613	1.00	8.55
3842	C	ALA	B	376	36.335	11.207	105.274	1.00	8.61
3843	O	ALA	B	376	36.429	10.358	106.150	1.00	9.01
3844	N	GLN	B	387	35.255	11.301	104.508	1.00	7.93
3846	CA	GLN	B	387	34.151	10.372	104.663	1.00	7.77
3848	CB	GLN	B	387	32.990	10.781	103.759	1.00	8.68
3851	CG	GLN	B	387	32.450	12.121	104.110	1.00	8.64
3854	CD	GLN	B	387	31.992	12.221	105.557	1.00	10.24
3855	OE1	GLN	B	387	31.279	11.334	106.059	1.00	11.05
3856	NE2	GLN	B	387	32.367	13.308	106.227	1.00	9.62
3859	C	GLN	B	387	34.585	8.950	104.356	1.00	8.78
3860	O	GLN	B	387	34.156	8.016	105.002	1.00	10.17
3861	N	LEU	B	398	35.445	8.786	103.372	1.00	8.57
3863	CA	LEU	B	398	35.952	7.465	103.000	1.00	9.27
3865	CB	LEU	B	398	36.815	7.561	101.737	1.00	9.86
3868	CG	LEU	B	398	37.406	6.251	101.236	1.00	11.50
3870	CD1	LEU	B	398	36.305	5.284	100.800	1.00	12.63

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3874	CD2	LEU	B	~~38~~———39	38.356	6.539	100.120	1.00	11.92
3878	C	LEU	B	39~~8~~	36.723	6.868	104.167	1.00	10.55
3879	O	LEU	B	39~~8~~	36.556	5.717	104.487	1.00	10.17
3880	N	LYS	B	40~~39~~	37.544	7.673	104.822	1.00	10.74
3882	CA	LYS	B	40~~39~~	38.277	7.203	105.991	1.00	11.40
3884	CB	LYS	B	40~~39~~	39.219	8.310	106.467	1.00	11.15
3887	CG	LYS	B	40~~39~~	39.948	7.973	107.784	1.00	11.85
3890	CD	LYS	B	40~~39~~	40.917	6.857	107.629	1.00	13.27
3893	CE	LYS	B	40~~39~~	41.569	6.576	108.974	1.00	15.75
3896	NZ	LYS	B	40~~39~~	42.653	5.537	108.883	1.00	19.28
3900	C	LYS	B	40~~39~~	37.328	6.810	107.118	1.00	11.94
3901	O	LYS	B	40~~39~~	37.523	5.771	107.757	1.00	12.56
3902	N	LEU	B	41~~0~~	36.300	7.617	107.376	1.00	12.13
3904	CA	LEU	B	41~~0~~	35.345	7.315	108.445	1.00	13.93
3906	CB	LEU	B	41~~0~~	34.377	8.467	108.634	1.00	14.19
3909	CG	LEU	B	41~~0~~	34.983	9.719	109.258	1.00	14.84
3911	CD1	LEU	B	41~~0~~	33.985	10.840	109.184	1.00	17.12
3915	CD2	LEU	B	41~~0~~	35.385	9.488	110.720	1.00	17.31
3919	C	LEU	B	41~~0~~	34.577	6.038	108.159	1.00	15.21
3920	O	LEU	B	41~~0~~	34.275	5.253	109.088	1.00	16.21
3921	N	ALA	B	42~~1~~	34.393	5.728	106.885	1.00	15.83
3923	CA	ALA	B	42~~1~~	33.529	4.628	106.516	1.00	17.19
3925	CB	ALA	B	42~~1~~	32.844	4.894	105.163	1.00	17.38
3929	C	ALA	B	42~~1~~	34.347	3.349	106.466	1.00	17.70
3930	O	ALA	B	42~~1~~	33.896	2.309	106.940	1.00	19.29
3931	N	THR	B	43~~2~~	35.567	3.422	105.933	1.00	16.91
3933	CA	THR	B	43~~2~~	36.348	2.220	105.653	1.00	16.81
3935	CB	THR	B	43~~2~~	36.749	2.177	104.162	1.00	17.11
3937	OG1	THR	B	43~~2~~	37.729	3.202	103.880	1.00	16.89
3939	CG2	THR	B	43~~2~~	35.572	2.466	103.279	1.00	18.75
3943	C	THR	B	43~~2~~	37.615	2.052	106.433	1.00	16.88
3944	O	THR	B	43~~2~~	38.232	0.967	106.399	1.00	17.65
3945	N	GLY	B	44~~3~~	38.059	3.119	107.075	1.00	15.64
3947	CA	GLY	B	44~~3~~	39.303	3.112	107.806	1.00	15.52
3950	C	GLY	B	44~~3~~	40.515	3.402	106.945	1.00	15.50
3951	O	GLY	B	44~~3~~	41.652	3.430	107.443	1.00	17.62
3952	N	ALA	B	45~~4~~	40.301	3.684	105.664	1.00	15.17
3954	CA	ALA	B	45~~4~~	41.423	3.919	104.789	1.00	14.36
3956	CB	ALA	B	45~~4~~	41.365	3.025	103.587	1.00	15.62
3960	C	ALA	B	45~~4~~	41.501	5.368	104.343	1.00	13.15
3961	O	ALA	B	45~~4~~	40.498	5.953	103.964	1.00	13.53
3962	N	LEU	B	46~~5~~	42.709	5.904	104.385	1.00	12.04
3964	CA	LEU	B	46~~5~~	42.968	7.265	103.947	1.00	11.39
3966	CB	LEU	B	46~~5~~	43.933	7.961	104.885	1.00	10.93
3969	CG	LEU	B	46~~5~~	44.127	9.445	104.559	1.00	12.26
3971	CD1	LEU	B	46~~5~~	42.825	10.262	104.667	1.00	12.42
3975	CD2	LEU	B	46~~5~~	45.194	10.024	105.486	1.00	13.92
3979	C	LEU	B	46~~5~~	43.563	7.199	102.544	1.00	11.65
3980	O	LEU	B	46~~5~~	44.690	6.734	102.344	1.00	12.63
3981	N	VAL	B	47~~6~~	42.794	7.665	101.568	1.00	11.14
3983	CA	VAL	B	47~~6~~	43.182	7.557	100.181	1.00	11.02

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
3985	CB	VAL	B	47~~6~~	42.297	6.511	99.450	1.00	11.66
3987	CG1	VAL	B	47~~6~~	42.718	6.383	97.993	1.00	13.42
3991	CG2	VAL	B	47~~6~~	42.360	5.192	100.152	1.00	14.64
3995	C	VAL	B	47~~6~~	42.942	8.867	99.477	1.00	10.49
3996	O	VAL	B	47~~6~~	41.832	9.406	99.549	1.00	11.57
3997	N	SER	B	48~~7~~	43.963	9.398	98.810	1.00	8.76
3999	CA	SER	B	48~~7~~	43.777	10.609	98.023	1.00	8.96
4001	CB	SER	B	48~~7~~	45.091	11.208	97.561	1.00	9.94
4004	OG	SER	B	48~~7~~	45.812	11.815	98.633	1.00	11.15
4006	C	SER	B	48~~7~~	42.924	10.243	96.828	1.00	9.05
4007	O	SER	B	48~~7~~	43.211	9.265	96.127	1.00	10.04
4008	N	LEU	B	49~~8~~	41.862	11.011	96.612	1.00	8.38
4010	CA	LEU	B	49~~8~~	40.940	10.763	95.494	1.00	8.52
4012	CB	LEU	B	49~~8~~	39.500	10.938	95.941	1.00	8.60
4015	CG	LEU	B	49~~8~~	39.103	9.978	97.050	1.00	7.65
4017	CD1	LEU	B	49~~8~~	37.729	10.289	97.575	1.00	9.76
4021	CD2	LEU	B	49~~8~~	39.156	8.535	96.551	1.00	9.85
4025	C	LEU	B	49~~8~~	41.294	11.670	94.333	1.00	8.59
4026	O	LEU	B	49~~8~~	41.989	12.669	94.477	1.00	9.68
4027	N	SER	B	50~~49~~	40.858	11.287	93.151	1.00	8.31
4029	CA	SER	B	50~~49~~	41.309	11.970	91.954	1.00	7.90
4031	CB	SER	B	50~~49~~	41.116	11.036	90.763	1.00	8.16
4034	OG	SER	B	50~~49~~	41.601	11.623	89.572	1.00	8.36
4036	C	SER	B	50~~49~~	40.623	13.286	91.629	1.00	8.57
4037	O	SER	B	50~~49~~	39.533	13.303	91.074	1.00	7.68
4038	N	ALA	B	51~~0~~	41.302	14.379	91.921	1.00	8.03
4040	CA	ALA	B	51~~0~~	40.818	15.679	91.509	1.00	8.81
4042	CB	ALA	B	51~~0~~	41.695	16.793	92.049	1.00	8.95
4046	C	ALA	B	51~~0~~	40.810	15.730	89.979	1.00	8.49
4047	O	ALA	B	51~~0~~	39.954	16.380	89.394	1.00	8.21
4048	N	GLN	B	52~~1~~	41.753	15.050	89.343	1.00	8.63
4050	CA	GLN	B	52~~1~~	41.798	15.051	87.881	1.00	8.65
4052	CB	GLN	B	52~~1~~	43.040	14.349	87.368	1.00	8.99
4055	CG	GLN	B	52~~1~~	43.223	14.579	85.870	1.00	9.63
4058	CD	GLN	B	52~~1~~	43.637	16.013	85.545	1.00	11.99
4059	OE1	GLN	B	52~~1~~	44.521	16.559	86.168	1.00	12.65
4060	NE2	GLN	B	52~~1~~	42.975	16.621	84.563	1.00	13.24
4063	C	GLN	B	52~~1~~	40.528	14.440	87.274	1.00	9.64
4064	O	GLN	B	52~~1~~	39.981	14.931	86.278	1.00	9.33
4065	N	ASN	B	53~~2~~	40.041	13.362	87.860	1.00	9.11
4067	CA	ASN	B	53~~2~~	38.810	12.714	87.458	1.00	9.28
4069	CB	ASN	B	53~~2~~	38.573	11.590	88.462	1.00	9.31
4072	CG	ASN	B	53~~2~~	37.448	10.649	88.137	1.00	9.37
4073	OD1	ASN	B	53~~2~~	37.393	9.605	88.755	1.00	11.21
4074	ND2	ASN	B	53~~2~~	36.506	11.012	87.280	1.00	10.32
4077	C	ASN	B	53~~2~~	37.664	13.729	87.460	1.00	9.51
4078	O	ASN	B	53~~2~~	36.845	13.755	86.531	1.00	9.76
4079	N	LEU	B	54~~3~~	37.615	14.596	88.461	1.00	8.97
4081	CA	LEU	B	54~~3~~	36.588	15.631	88.494	1.00	10.39
4083	CB	LEU	B	54~~3~~	36.584	16.350	89.818	1.00	9.70
4086	CG	LEU	B	54~~3~~	35.558	15.949	90.881	1.00	16.46

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4088	CD1	LEU	B	543	34.797	14.670	90.688	1.00	12.87
4092	CD2	LEU	B	543	36.061	16.166	92.304	1.00	11.64
4096	C	LEU	B	543	36.806	16.642	87.379	1.00	9.86
4097	O	LEU	B	543	35.850	16.994	86.659	1.00	10.00
4098	N	VAL	B	554	38.031	17.123	87.235	1.00	9.33
4100	CA	VAL	B	554	38.347	18.116	86.219	1.00	9.99
4102	CB	VAL	B	554	39.842	18.449	86.256	1.00	9.74
4104	CG1	VAL	B	554	40.286	19.212	85.018	1.00	11.28
4108	CG2	VAL	B	554	40.143	19.252	87.456	1.00	12.01
4112	C	VAL	B	554	37.936	17.614	84.836	1.00	10.31
4113	O	VAL	B	554	37.351	18.361	84.048	1.00	11.19
4114	N	ASP	B	565	38.246	16.360	84.549	1.00	11.19
4116	CA	ASP	B	565	38.039	15.795	83.226	1.00	11.46
4118	CB	ASP	B	565	38.933	14.576	83.041	1.00	11.64
4121	CG	ASP	B	565	40.405	14.890	83.055	1.00	13.05
4122	OD1	ASP	B	565	40.835	16.070	82.982	1.00	14.37
4123	OD2	ASP	B	565	41.248	13.962	83.109	1.00	14.70
4124	C	ASP	B	565	36.641	15.305	82.957	1.00	12.09
4125	O	ASP	B	565	36.216	15.218	81.793	1.00	13.10
4126	N	CYS	B	576	35.948	14.880	84.001	1.00	12.05
4128	CA	CYS	B	576	34.683	14.184	83.830	1.00	12.46
4130	CB	CYS	B	576	34.747	12.788	84.452	1.00	12.56
4133	SG	CYS	B	576	36.201	11.822	83.971	1.00	15.36
4134	C	CYS	B	576	33.459	14.897	84.348	1.00	12.46
4135	O	CYS	B	576	32.375	14.672	83.849	1.00	13.79
4136	N	SER	B	587	33.600	15.710	85.387	1.00	11.17
4138	CA	SER	B	587	32.498	16.478	85.911	1.00	11.43
4140	CB	SER	B	587	32.632	16.649	87.416	1.00	11.27
4143	OG	SER	B	587	31.548	17.370	87.938	1.00	11.40
4145	C	SER	B	587	32.586	17.808	85.209	1.00	11.42
4146	O	SER	B	587	33.053	18.786	85.762	1.00	11.26
4147	N	THR	B	598	32.138	17.808	83.963	1.00	11.59
4149	CA	THR	B	598	32.349	18.947	83.092	1.00	12.31
4151	CB	THR	B	598	33.063	18.484	81.838	1.00	12.81
4153	OG1	THR	B	598	32.391	17.341	81.284	1.00	14.54
4155	CG2	THR	B	598	34.500	18.021	82.177	1.00	13.07
4159	C	THR	B	598	31.061	19.698	82.764	1.00	12.11
4160	O	THR	B	598	30.321	20.052	83.650	1.00	11.59
4161	N	GLU	B	6059	30.797	19.951	81.483	1.00	13.48
4163	CA	GLU	B	6059	29.624	20.748	81.078	1.00	15.01
4165	CB	GLU	B	6059	29.505	20.703	79.559	1.00	15.79
4168	CG	GLU	B	6059	30.629	21.404	78.840	1.00	21.29
4171	CD	GLU	B	6059	31.731	20.461	78.374	1.00	26.19
4172	OE1	GLU	B	6059	31.930	19.394	79.001	1.00	26.04
4173	OE2	GLU	B	6059	32.396	20.812	77.371	1.00	31.07
4174	C	GLU	B	6059	28.254	20.394	81.660	1.00	13.56
4175	O	GLU	B	6059	27.494	21.283	82.052	1.00	13.00
4176	N	ALA	B	610	28.021	19.141	81.954	1.00	13.64
4178	CA	ALA	B	610	26.702	18.677	82.295	1.00	12.46
4180	CB	ALA	B	610	26.481	17.195	82.026	1.00	14.54
4184	C	ALA	B	610	26.533	19.014	83.774	1.00	11.82

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4185	O	ALA	B	610	25.433	19.099	84.259	1.00	12.79
4186	N	TYR	B	621	27.653	19.292	84.443	1.00	10.69
4188	CA	TYR	B	621	27.659	19.640	85.855	1.00	9.57
4190	CB	TYR	B	621	28.670	18.742	86.595	1.00	8.42
4193	CG	TYR	B	621	28.178	17.325	86.563	1.00	9.60
4194	CD1	TYR	B	621	28.565	16.441	85.581	1.00	8.86
4196	CE1	TYR	B	621	28.032	15.166	85.525	1.00	9.12
4198	CZ	TYR	B	621	27.115	14.777	86.455	1.00	8.99
4199	OH	TYR	B	621	26.549	13.529	86.458	1.00	13.09
4201	CE2	TYR	B	621	26.715	15.631	87.411	1.00	8.13
4203	CD2	TYR	B	621	27.228	16.898	87.462	1.00	9.81
4205	C	TYR	B	621	27.956	21.109	86.075	1.00	9.66
4206	O	TYR	B	621	28.184	21.574	87.189	1.00	9.26
4207	N	GLY	B	632	27.934	21.865	84.979	1.00	9.48
4209	CA	GLY	B	632	28.173	23.287	85.083	1.00	10.21
4212	C	GLY	B	632	29.616	23.653	85.363	1.00	10.62
4213	O	GLY	B	632	29.908	24.813	85.655	1.00	11.37
4214	N	ASN	B	643	30.516	22.676	85.250	1.00	10.40
4216	CA	ASN	B	643	31.931	22.890	85.523	1.00	11.35
4218	CB	ASN	B	643	32.512	21.709	86.299	1.00	10.23
4221	CG	ASN	B	643	31.815	21.486	87.610	1.00	10.37
4222	OD1	ASN	B	643	31.643	20.330	88.047	1.00	12.69
4223	ND2	ASN	B	643	31.355	22.552	88.218	1.00	8.16
4226	C	ASN	B	643	32.751	23.120	84.256	1.00	12.10
4227	O	ASN	B	643	32.422	22.619	83.187	1.00	13.78
4228	N	ALA	B	654	33.859	23.829	84.423	1.00	12.86
4230	CA	ALA	B	654	34.723	24.232	83.330	1.00	13.97
4232	CB	ALA	B	654	34.706	25.762	83.207	1.00	15.21
4236	C	ALA	B	654	36.154	23.757	83.508	1.00	14.13
4237	O	ALA	B	654	37.073	24.366	82.982	1.00	15.28
4238	N	GLY	B	665	36.355	22.676	84.256	1.00	13.80
4240	CA	GLY	B	665	37.675	22.113	84.411	1.00	14.33
4243	C	GLY	B	665	38.639	23.076	85.060	1.00	14.48
4244	O	GLY	B	665	38.443	23.568	86.179	1.00	14.34
4245	N	CYS	B	676	39.715	23.369	84.349	1.00	15.50
4247	CA	CYS	B	676	40.714	24.266	84.882	1.00	16.73
4249	CB	CYS	B	676	41.991	24.179	84.063	1.00	17.47
4252	SG	CYS	B	676	42.870	22.637	84.376	1.00	21.35
4253	C	CYS	B	676	40.224	25.707	84.914	1.00	17.09
4254	O	CYS	B	676	40.927	26.591	85.382	1.00	17.41
4255	N	ASN	B	687	39.022	25.932	84.415	1.00	17.06
4257	CA	ASN	B	687	38.444	27.251	84.477	1.00	18.11
4259	CB	ASN	B	687	38.041	27.719	83.093	1.00	18.35
4262	CG	ASN	B	687	39.231	28.143	82.298	1.00	23.44
4263	OD1	ASN	B	687	39.907	29.121	82.657	1.00	27.10
4264	ND2	ASN	B	687	39.554	27.383	81.257	1.00	26.80
4267	C	ASN	B	687	37.306	27.361	85.469	1.00	17.92
4268	O	ASN	B	687	36.448	28.220	85.350	1.00	19.56
4269	N	GLY	B	698	37.318	26.500	86.470	1.00	15.88
4271	CA	GLY	B	698	36.372	26.605	87.557	1.00	14.83
4274	C	GLY	B	698	35.225	25.625	87.564	1.00	13.38

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4275	O	GLY	B	69~~8~~	34.821	25.064	86.545	1.00	13.78
4276	N	GLY	B	70~~69~~	34.679	25.435	88.750	1.00	11.45
4278	CA	GLY	B	70~~69~~	33.568	24.535	88.917	1.00	10.88
4281	C	GLY	B	70~~69~~	32.988	24.660	90.302	1.00	9.57
4282	O	GLY	B	70~~69~~	33.331	25.577	91.032	1.00	11.25
4283	N	PHE	B	71~~0~~	32.130	23.706	90.659	1.00	8.89
4285	CA	PHE	B	71~~0~~	31.426	23.680	91.935	1.00	8.32
4287	CB	PHE	B	71~~0~~	29.913	23.772	91.698	1.00	8.55
4290	CG	PHE	B	71~~0~~	29.478	24.990	90.940	1.00	10.94
4291	CD1	PHE	B	71~~0~~	29.187	24.916	89.605	1.00	11.01
4293	CE1	PHE	B	71~~0~~	28.753	26.055	88.913	1.00	15.77
4295	CZ	PHE	B	71~~0~~	28.595	27.225	89.582	1.00	16.23
4297	CE2	PHE	B	71~~0~~	28.881	27.302	90.908	1.00	16.21
4299	CD2	PHE	B	71~~0~~	29.309	26.173	91.590	1.00	14.41
4301	C	PHE	B	71~~0~~	31.672	22.375	92.671	1.00	8.19
4302	O	PHE	B	71~~0~~	31.660	21.316	92.073	1.00	8.98
4303	N	MET	B	72~~1~~	31.851	22.446	93.986	1.00	7.88
4305	CA	MET	B	72~~1~~	32.012	21.256	94.792	1.00	7.85
4307	CB	MET	B	72~~1~~	32.459	21.596	96.209	1.00	7.97
4310	CG	MET	B	72~~1~~	33.853	22.147	96.295	1.00	9.20
4313	SD	MET	B	72~~1~~	34.004	23.905	95.949	1.00	10.32
4314	CE	MET	B	72~~1~~	33.363	24.566	97.447	1.00	10.98
4318	C	MET	B	72~~1~~	30.739	20.443	94.833	1.00	7.62
4319	O	MET	B	72~~1~~	30.782	19.216	94.756	1.00	7.54
4320	N	THR	B	73~~2~~	29.605	21.129	94.948	1.00	8.53
4322	CA	THR	B	73~~2~~	28.343	20.412	95.022	1.00	8.73
4324	CB	THR	B	73~~2~~	27.185	21.343	95.266	1.00	9.57
4326	OG1	THR	B	73~~2~~	27.275	22.421	94.342	1.00	11.50
4328	CG2	THR	B	73~~2~~	27.253	21.976	96.650	1.00	10.28
4332	C	THR	B	73~~2~~	28.085	19.597	93.758	1.00	8.32
4333	O	THR	B	73~~2~~	27.636	18.450	93.862	1.00	9.16
4334	N	THR	B	74~~3~~	28.329	20.190	92.577	1.00	8.20
4336	CA	THR	B	74~~3~~	28.059	19.470	91.352	1.00	8.05
4338	CB	THR	B	74~~3~~	27.917	20.383	90.134	1.00	8.06
4340	OG1	THR	B	74~~3~~	29.199	20.870	89.765	1.00	8.32
4342	CG2	THR	B	74~~3~~	27.086	21.594	90.453	1.00	8.91
4346	C	THR	B	74~~3~~	29.112	18.393	91.131	1.00	8.37
4347	O	THR	B	74~~3~~	28.833	17.397	90.466	1.00	9.64
4348	N	ALA	B	75~~4~~	30.321	18.591	91.665	1.00	8.05
4350	CA	ALA	B	75~~4~~	31.305	17.526	91.690	1.00	8.09
4352	CB	ALA	B	75~~4~~	32.620	18.006	92.247	1.00	8.30
4356	C	ALA	B	75~~4~~	30.768	16.328	92.493	1.00	8.31
4357	O	ALA	B	75~~4~~	30.873	15.192	92.027	1.00	8.21
4358	N	PHE	B	76~~5~~	30.182	16.572	93.672	1.00	7.60
4360	CA	PHE	B	76~~5~~	29.592	15.506	94.501	1.00	7.71
4362	CB	PHE	B	76~~5~~	29.022	16.048	95.803	1.00	7.65
4365	CG	PHE	B	76~~5~~	30.026	16.650	96.727	1.00	7.26
4366	CD1	PHE	B	76~~5~~	31.284	16.079	96.914	1.00	8.91
4368	CE1	PHE	B	76~~5~~	32.178	16.659	97.774	1.00	8.41
4370	CZ	PHE	B	76~~5~~	31.823	17.768	98.493	1.00	7.23
4372	CE2	PHE	B	76~~5~~	30.580	18.329	98.339	1.00	7.15

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4374	CD2	PHE	B	76~~5~~	29.681	17.764	97.459	1.00	7.67
4376	C	PHE	B	76~~5~~	28.492	14.753	93.761	1.00	8.67
4377	O	PHE	B	76~~5~~	28.404	13.523	93.859	1.00	9.55
4378	N	GLN	B	77~~6~~	27.618	15.517	93.076	1.00	8.33
4380	CA	GLN	B	77~~6~~	26.566	14.931	92.235	1.00	7.96
4382	CB	GLN	B	77~~6~~	25.585	15.978	91.691	1.00	8.51
4385	CG	GLN	B	77~~6~~	24.377	15.319	91.068	1.00	8.97
4388	CD	GLN	B	77~~6~~	23.543	14.582	92.087	1.00	10.92
4389	OE1	GLN	B	77~~6~~	23.325	15.073	93.198	1.00	12.07
4390	NE2	GLN	B	77~~6~~	23.064	13.399	91.719	1.00	11.85
4393	C	GLN	B	77~~6~~	27.131	14.080	91.094	1.00	7.30
4394	O	GLN	B	77~~6~~	26.573	13.022	90.799	1.00	9.51
4395	N	TYR	B	78~~7~~	28.204	14.516	90.457	1.00	8.18
4397	CA	TYR	B	78~~7~~	28.848	13.702	89.422	1.00	7.77
4399	CB	TYR	B	78~~7~~	30.048	14.398	88.781	1.00	8.35
4402	CG	TYR	B	78~~7~~	30.998	13.432	88.138	1.00	8.06
4403	CD1	TYR	B	78~~7~~	30.792	12.958	86.849	1.00	10.38
4405	CE1	TYR	B	78~~7~~	31.671	12.044	86.275	1.00	10.92
4407	CZ	TYR	B	78~~7~~	32.756	11.573	87.004	1.00	9.98
4408	OH	TYR	B	78~~7~~	33.639	10.675	86.424	1.00	11.11
4410	CE2	TYR	B	78~~7~~	32.968	12.051	88.283	1.00	10.78
4412	CD2	TYR	B	78~~7~~	32.091	12.949	88.834	1.00	9.09
4414	C	TYR	B	78~~7~~	29.277	12.368	90.020	1.00	8.25
4415	O	TYR	B	78~~7~~	29.062	11.312	89.426	1.00	8.42
4416	N	ILE	B	79~~8~~	29.909	12.405	91.192	1.00	8.19
4418	CA	ILE	B	79~~8~~	30.357	11.148	91.803	1.00	8.50
4420	CB	ILE	B	79~~8~~	31.114	11.408	93.136	1.00	8.00
4422	CG1	ILE	B	79~~8~~	32.314	12.325	92.895	1.00	9.06
4425	CD1	ILE	B	79~~8~~	33.058	12.711	94.130	1.00	8.90
4429	CG2	ILE	B	79~~8~~	31.602	10.109	93.745	1.00	9.03
4433	C	ILE	B	79~~8~~	29.155	10.252	92.055	1.00	8.48
4434	O	ILE	B	79~~8~~	29.207	9.031	91.839	1.00	9.49
4435	N	ILE	B	80~~79~~	28.074	10.830	92.552	1.00	8.13
4437	CA	ILE	B	80~~79~~	26.841	10.066	92.808	1.00	9.58
4439	CB	ILE	B	80~~79~~	25.765	10.937	93.483	1.00	10.42
4441	CG1	ILE	B	80~~79~~	26.244	11.493	94.820	1.00	10.50
4444	CD1	ILE	B	80~~79~~	25.401	12.643	95.340	1.00	11.47
4448	CG2	ILE	B	80~~79~~	24.461	10.156	93.722	1.00	10.69
4452	C	ILE	B	80~~79~~	26.310	9.477	91.491	1.00	10.18
4453	O	ILE	B	80~~79~~	26.091	8.267	91.383	1.00	11.75
4454	N	ASP	B	81~~0~~	26.154	10.322	90.478	1.00	9.99
4456	CA	ASP	B	81~~0~~	25.629	9.879	89.177	1.00	10.47
4458	CB	ASP	B	81~~0~~	25.536	11.066	88.225	1.00	10.84
4461	CG	ASP	B	81~~0~~	24.485	12.051	88.629	1.00	11.63
4462	OD1	ASP	B	81~~0~~	24.498	13.178	88.045	1.00	14.19
4463	OD2	ASP	B	81~~0~~	23.626	11.789	89.489	1.00	13.10
4464	C	ASP	B	81~~0~~	26.519	8.846	88.521	1.00	11.15
4465	O	ASP	B	81~~0~~	26.030	7.908	87.882	1.00	12.20
4466	N	ASN	B	82~~1~~	27.825	9.026	88.666	1.00	10.79
4468	CA	ASN	B	82~~1~~	28.826	8.200	88.021	1.00	10.42
4470	CB	ASN	B	82~~1~~	30.141	8.964	87.980	1.00	10.26

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4473	CG	ASN	B	821	31.163	8.316	87.073	1.00	11.69
4474	OD1	ASN	B	821	30.895	8.082	85.874	1.00	12.68
4475	ND2	ASN	B	821	32.342	8.032	87.610	1.00	12.51
4478	C	ASN	B	821	29.063	6.887	88.748	1.00	10.42
4479	O	ASN	B	821	29.714	5.992	88.196	1.00	11.10
4480	N	LYS	B	832	28.531	6.794	89.960	1.00	10.79
4482	CA	LYS	B	832	28.691	5.655	90.855	1.00	12.12
4484	CB	LYS	B	832	28.063	4.387	90.274	1.00	13.64
4487	CG	LYS	B	832	26.592	4.558	89.929	1.00	16.00
4490	CD	LYS	B	832	25.923	3.218	89.692	1.00	21.87
4493	CE	LYS	B	832	24.466	3.356	89.234	1.00	24.58
4496	NZ	LYS	B	832	23.671	4.285	90.077	1.00	28.17
4500	C	LYS	B	832	30.147	5.427	91.228	1.00	11.97
4501	O	LYS	B	832	30.576	4.278	91.453	1.00	12.61
4502	N	GLY	B	843	30.926	6.505	91.297	1.00	10.76
4504	CA	GLY	B	843	32.289	6.392	91.755	1.00	10.12
4507	C	GLY	B	843	33.218	7.493	91.340	1.00	9.65
4508	O	GLY	B	843	32.926	8.297	90.461	1.00	10.02
4509	N	ILE	B	854	34.380	7.492	91.981	1.00	8.48
4511	CA	ILE	B	854	35.482	8.338	91.631	1.00	8.25
4513	CB	ILE	B	854	35.530	9.639	92.497	1.00	6.86
4515	CG1	ILE	B	854	36.682	10.516	92.049	1.00	8.42
4518	CD1	ILE	B	854	36.640	11.925	92.665	1.00	9.75
4522	CG2	ILE	B	854	35.623	9.294	93.977	1.00	8.15
4526	C	ILE	B	854	36.761	7.499	91.822	1.00	8.41
4527	O	ILE	B	854	36.922	6.806	92.828	1.00	9.82
4528	N	ASP	B	865	37.696	7.690	90.914	1.00	8.81
4530	CA	ASP	B	865	38.962	6.965	90.935	1.00	8.24
4532	CB	ASP	B	865	39.609	6.993	89.560	1.00	8.96
4535	CG	ASP	B	865	38.873	6.150	88.560	1.00	8.27
4536	OD1	ASP	B	865	38.150	5.188	88.950	1.00	9.46
4537	OD2	ASP	B	865	39.004	6.415	87.352	1.00	9.81
4538	C	ASP	B	865	39.918	7.526	91.979	1.00	9.50
4539	O	ASP	B	865	39.775	8.658	92.430	1.00	8.14
4540	N	SER	B	876	40.856	6.699	92.430	1.00	9.34
4542	CA	SER	B	876	41.847	7.181	93.386	1.00	10.67
4544	CB	SER	B	876	42.615	6.043	94.040	1.00	11.08
4547	OG	SER	B	876	43.430	5.536	93.057	1.00	13.75
4549	C	SER	B	876	42.812	8.114	92.635	1.00	10.27
4550	O	SER	B	876	42.974	8.046	91.370	1.00	8.88
4551	N	ASP	B	887	43.439	9.013	93.392	1.00	10.36
4553	CA	ASP	B	887	44.504	9.875	92.869	1.00	11.49
4555	CB	ASP	B	887	45.006	10.769	94.026	1.00	11.83
4558	CG	ASP	B	887	46.186	11.638	93.649	1.00	16.32
4559	OD1	ASP	B	887	45.974	12.611	92.887	1.00	20.70
4560	OD2	ASP	B	887	47.327	11.483	94.116	1.00	22.95
4561	C	ASP	B	887	45.626	9.043	92.194	1.00	10.94
4562	O	ASP	B	887	46.111	9.347	91.109	1.00	11.59
4563	N	ALA	B	898	46.027	7.965	92.842	1.00	10.32
4565	CA	ALA	B	898	47.107	7.117	92.306	1.00	10.44
4567	CB	ALA	B	898	47.426	6.043	93.323	1.00	11.26

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4571	C	ALA	B	898	46.828	6.499	90.924	1.00	11.67
4573	N	SER	B	9089	45.558	6.206	90.673	1.00	10.71
4575	CA	SER	B	9089	45.171	5.613	89.390	1.00	11.12
4577	CB	SER	B	9089	43.904	4.782	89.559	1.00	11.37
4580	OG	SER	B	9089	42.754	5.600	89.697	1.00	13.11
4582	C	SER	B	9089	44.886	6.659	88.333	1.00	11.23
4583	O	SER	B	9089	44.956	6.390	87.137	1.00	12.38
4584	N	TYR	B	910	44.551	7.868	88.773	1.00	11.41
4586	CA	TYR	B	910	44.112	8.915	87.850	1.00	10.61
4588	CB	TYR	B	910	42.584	8.980	87.870	1.00	9.85
4591	CG	TYR	B	910	41.910	9.681	86.733	1.00	10.08
4592	CD1	TYR	B	910	42.566	10.649	86.019	1.00	10.98
4594	CE1	TYR	B	910	41.955	11.283	84.986	1.00	10.52
4596	CZ	TYR	B	910	40.658	10.927	84.702	1.00	11.69
4597	OH	TYR	B	910	40.058	11.605	83.638	1.00	13.78
4600	CD2	TYR	B	910	40.605	9.376	86.424	1.00	10.93
4601	C	TYR	B	910	44.757	10.212	88.360	1.00	10.48
4602	O	TYR	B	910	44.107	11.049	88.957	1.00	10.15
4603	N	PRO	B	921	46.062	10.346	88.168	1.00	11.68
4604	CA	PRO	B	921	46.838	11.446	88.741	1.00	11.88
4606	CB	PRO	B	921	48.290	11.045	88.465	1.00	12.35
4609	CG	PRO	B	921	48.255	9.910	87.567	1.00	14.21
4612	CD	PRO	B	921	.46.888	9.436	87.364	1.00	12.70
4615	C	PRO	B	921	46.551	12.807	88.148	1.00	11.76
4616	O	PRO	B	921	46.024	12.965	87.041	1.00	10.77
4617	N	TYR	B	932	46.898	13.810	88.931	1.00	11.47
4619	CA	TYR	B	932	46.624	15.197	88.617	1.00	11.76
4621	CB	TYR	B	932	46.532	15.984	89.910	1.00	11.22
4624	CG	TYR	B	932	46.198	17.436	89.691	1.00	10.65
4625	CD1	TYR	B	932	44.922	17.817	89.308	1.00	11.18
4627	CE1	TYR	B	932	44.609	19.127	89.115	1.00	11.70
4629	CZ	TYR	B	932	45.571	20.087	89.307	1.00	9.89
4630	OH	TYR	B	932	45.234	21.409	89.126	1.00	11.27
4632	CE2	TYR	B	932	46.849	19.733	89.676	1.00	10.31
4634	CD2	TYR	B	932	47.147	18.409	89.863	1.00	10.28
4636	C	TYR	B	932	47.691	15.796	87.725	1.00	12.10
4637	O	TYR	B	932	48.898	15.725	88.023	1.00	13.64
4638	N	LYS	B	943	47.228	16.397	86.637	1.00	13.23
4640	CA	LYS	B	943	48.100	16.918	85.603	1.00	14.76
4642	CB	LYS	B	943	47.817	16.206	84.273	1.00	16.16
4645	CG	LYS	B	943	47.968	14.679	84.325	1.00	19.21
4648	CD	LYS	B	943	49.374	14.247	84.575	1.00	23.76
4651	CE	LYS	B	943	49.509	12.722	84.524	1.00	26.95
4654	NZ	LYS	B	943	50.893	12.279	84.844	1.00	29.84
4658	C	LYS	B	943	47.964	18.427	85.420	1.00	15.08
4659	O	LYS	B	943	48.675	19.016	84.627	1.00	15.38
4660	N	ALA	B	954	47.037	19.047	86.131	1.00	15.07
4662	CA	ALA	B	954	46.877	20.507	86.071	1.00	15.34
4664	CB	ALA	B	954	48.113	21.224	86.609	1.00	15.03
4668	C	ALA	B	954	46.552	20.988	84.664	1.00	15.73
4669	O	ALA	B	954	47.050	22.018	84.205	1.00	16.56

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4670	N	MET	B	96~~5~~	45.670	20.257	84.015	1.00	16.35
4672	CA	MET	B	96~~5~~	45.178	20.611	82.693	1.00	17.55
4674	CB	MET	B	96~~5~~	46.227	20.346	81.617	1.00	18.91
4677	CG	MET	B	96~~5~~	46.512	18.893	81.356	1.00	21.90
4680	SD	MET	B	96~~5~~	47.975	18.650	80.240	1.00	30.57
4681	CE	MET	B	96~~5~~	48.879	20.074	80.606	1.00	27.93
4685	C	MET	B	96~~5~~	43.909	19.843	82.404	1.00	17.30
4686	O	MET	B	96~~5~~	43.635	18.831	83.041	1.00	17.10
4687	N	ASP	B	97~~6~~	43.109	20.344	81.469	1.00	17.36
4689	CA	ASP	B	97~~6~~	41.900	19.663	81.049	1.00	17.45
4691	CB	ASP	B	97~~6~~	40.989	20.589	80.234	1.00	17.93
4694	CG	ASP	B	97~~6~~	40.430	21.737	81.041	1.00	20.60
4695	OD1	ASP	B	97~~6~~	40.298	22.834	80.458	1.00	27.70
4696	OD2	ASP	B	97~~6~~	40.082	21.651	82.232	1.00	22.07
4697	C	ASP	B	97~~6~~	42.291	18.490	80.177	1.00	17.57
4698	O	ASP	B	97~~6~~	43.129	18.646	79.291	1.00	17.89
4699	N	GLN	B	98~~7~~	41.674	17.341	80.424	1.00	17.20
4701	CA	GLN	B	98~~7~~	41.887	16.113	79.638	1.00	17.41
4703	CB	GLN	B	98~~7~~	42.715	15.094	80.430	1.00	17.50
4706	CG	GLN	B	98~~7~~	43.968	15.638	81.018	1.00	18.00
4709	CD	GLN	B	98~~7~~	44.726	14.586	81.818	1.00	19.25
4710	OE1	GLN	B	98~~7~~	44.113	13.767	82.536	1.00	21.54
4711	NE2	GLN	B	98~~7~~	46.047	14.603	81.713	1.00	19.05
4714	C	GLN	B	98~~7~~	40.560	15.482	79.297	1.00	17.51
4715	O	GLN	B	98~~7~~	39.518	15.832	79.861	1.00	17.06
4716	N	ALA	B	99~~8~~	40.624	14.407	78.518	1.00	18.52
4718	CA	ALA	B	99~~8~~	39.435	13.705	78.079	1.00	18.69
4720	CB	ALA	B	99~~8~~	39.733	12.731	76.936	1.00	19.79
4724	C	ALA	B	99~~8~~	39.056	12.920	79.307	1.00	17.88
4725	O	ALA	B	99~~8~~	39.937	12.539	80.083	1.00	18.71
4726	N	CYS	B	100~~99~~	37.768	12.689	79.478	1.00	18.05
4728	CA	CYS	B	100~~99~~	37.291	11.862	80.555	1.00	18.44
4730	CB	CYS	B	100~~99~~	35.794	11.704	80.451	1.00	18.49
4733	SG	CYS	B	100~~99~~	35.170	10.501	81.619	1.00	25.88
4734	C	CYS	B	100~~99~~	37.930	10.494	80.440	1.00	16.92
4735	O	CYS	B	100~~99~~	37.794	9.843	79.411	1.00	16.03
4736	N	GLN	B	101~~0~~	38.636	10.063	81.487	1.00	15.03
4738	CA	GLN	B	101~~0~~	39.259	8.736	81.508	1.00	14.98
4740	CB	GLN	B	101~~0~~	40.766	8.863	81.435	1.00	15.56
4743	CG	GLN	B	101~~0~~	41.250	9.511	80.158	1.00	19.02
4746	CD	GLN	B	101~~0~~	42.597	10.174	80.326	1.00	22.86
4747	OE1	GLN	B	101~~0~~	42.683	11.375	80.634	1.00	27.00
4748	NE2	GLN	B	101~~0~~	43.656	9.406	80.109	1.00	25.05
4751	C	GLN	B	101~~0~~	38.851	7.921	82.731	1.00	13.31
4752	O	GLN	B	101~~0~~	39.564	6.993	83.145	1.00	13.56
4753	N	TYR	B	102~~1~~	37.707	8.243	83.308	1.00	12.42
4755	CA	TYR	B	102~~1~~	37.213	7.495	84.437	1.00	11.79
4757	CB	TYR	B	102~~1~~	35.847	7.976	84.888	1.00	11.62
4760	CG	TYR	B	102~~1~~	35.269	7.084	85.945	1.00	10.52
4761	CD1	TYR	B	102~~1~~	35.694	7.177	87.263	1.00	8.99
4763	CE1	TYR	B	102~~1~~	35.189	6.364	88.212	1.00	10.14

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4765	CZ	TYR	B	1021	34.237	5.430	87.894	1.00	10.37
4766	OH	TYR	B	1021	33.735	4.602	88.865	1.00	11.45
4768	CE2	TYR	B	1021	33.803	5.304	86.568	1.00	10.21
4770	CD2	TYR	B	1021	34.338	6.116	85.623	1.00	10.30
4772	C	TYR	B	1021	37.120	6.025	84.058	1.00	12.30
4773	O	TYR	B	1021	36.644	5.675	82.971	1.00	13.41
4774	N	ASP	B	1022	37.466	5.159	84.996	1.00	12.26
4776	CA	ASP	B	1032	37.343	3.726	84.799	1.00	13.19
4778	CB	ASP	B	1032	38.620	3.086	84.313	1.00	13.30
4781	CG	ASP	B	1032	38.376	1.702	83.732	1.00	15.06
4782	OD1	ASP	B	1032	37.634	0.916	84.344	1.00	14.48
4783	OD2	ASP	B	1032	38.862	1.357	82.636	1.00	20.41
4784	C	ASP	B	1032	36.930	3.166	86.119	1.00	12.83
4785	O	ASP	B	1032	37.604	3.394	87.128	1.00	12.67
4786	N	SER	B	1043	35.813	2.462	86.148	1.00	12.16
4788	CA	SER	B	1043	35.313	1.899	87.394	1.00	11.91
4790	CB	SER	B	1043	33.975	1.198	87.239	1.00	12.80
4793	OG	SER	B	1043	34.087	0.078	86.362	1.00	15.16
4795	C	SER	B	1043	36.309	0.918	88.003	1.00	10.68
4796	O	SER	B	1043	36.242	0.642	89.178	1.00	11.66
4797	N	LYS	B	1054	37.200	0.352	87.199	1.00	10.52
4799	CA	LYS	B	1054	38.152	-0.601	87.777	1.00	9.41
4801	CB	LYS	B	1054	38.918	-1.402	86.724	1.00	9.47
4804	CG	LYS	B	1054	39.975	-0.658	86.000	1.00	8.88
4807	CD	LYS	B	1054	40.513	-1.392	84.758	1.00	9.76
4810	CE	LYS	B	1054	41.556	-0.617	84.028	1.00	12.01
4813	NZ	LYS	B	1054	41.898	-1.250	82.689	1.00	14.12
4817	C	LYS	B	1054	39.119	0.082	88.736	1.00	9.62
4818	O	LYS	B	1054	39.802	-0.579	89.507	1.00	10.38
4819	N	TYR	B	1065	39.158	1.411	88.702	1.00	9.13
4821	CA	TYR	B	1065	40.022	2.175	89.606	1.00	9.12
4823	CB	TYR	B	1065	40.890	3.149	88.822	1.00	9.76
4826	CG	TYR	B	1065	41.857	2.510	87.844	1.00	11.14
4827	CD1	TYR	B	1065	42.042	3.044	86.599	1.00	13.82
4829	CE1	TYR	B	1065	42.950	2.497	85.715	1.00	14.78
4831	CZ	TYR	B	1065	43.669	1.378	86.083	1.00	14.11
4832	OH	TYR	B	1065	44.569	0.849	85.181	1.00	15.45
4834	CE2	TYR	B	1065	43.514	0.840	87.331	1.00	11.85
4836	CD2	TYR	B	1065	42.620	1.416	88.206	1.00	11.84
4838	C	TYR	B	1065	39.219	2.930	90.672	1.00	8.87
4839	O	TYR	B	1065	39.768	3.794	91.367	1.00	9.98
4840	N	ARG	B	1076	37.974	2.568	90.816	1.00	9.03
4842	CA	ARG	B	1076	37.108	3.209	91.798	1.00	9.75
4844	CB	ARG	B	1076	35.693	2.701	91.701	1.00	9.91
4847	CG	ARG	B	1076	34.747	3.363	92.657	1.00	12.62
4850	CD	ARG	B	1076	33.522	2.547	92.909	1.00	19.23
4853	NE	ARG	B	1076	32.776	2.354	91.678	1.00	24.16
4855	CZ	ARG	B	1076	32.387	1.179	91.184	1.00	27.02
4856	NH1	ARG	B	1076	32.672	0.042	91.812	1.00	29.58
4859	NH2	ARG	B	1076	31.701	1.147	90.044	1.00	26.59
4862	C	ARG	B	1076	37.612	3.038	93.232	1.00	10.74

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4863	O	ARG	B	1076	37.843	1.928	93.727	1.00	11.98
4864	N	ALA	B	1087	37.640	4.189	93.913	1.00	10.07
4866	CA	ALA	B	1087	38.161	4.235	95.262	1.00	9.59
4868	CB	ALA	B	1087	39.413	5.099	95.354	1.00	10.32
4872	C	ALA	B	1087	37.144	4.749	96.223	1.00	10.28
4873	O	ALA	B	1087	37.313	4.577	97.422	1.00	11.26
4874	N	ALA	B	1098	36.100	5.412	95.729	1.00	9.38
4876	CA	ALA	B	1098	35.076	5.936	96.605	1.00	9.81
4878	CB	ALA	B	1098	35.465	7.306	97.176	1.00	9.71
4882	C	ALA	B	1098	33.789	6.086	95.842	1.00	9.71
4883	O	ALA	B	1098	33.783	6.144	94.627	1.00	10.32
4884	N	THR	B	10109	32.712	6.159	96.584	1.00	10.66
4886	CA	THR	B	11009	31.389	6.453	96.067	1.00	10.67
4888	CB	THR	B	11009	30.460	5.222	96.148	1.00	10.94
4890	OG1	THR	B	11009	30.335	4.782	97.511	1.00	12.67
4892	CG2	THR	B	11009	31.034	4.065	95.373	1.00	13.43
4896	C	THR	B	11009	30.824	7.563	96.935	1.00	11.09
4897	O	THR	B	11009	31.383	7.921	97.967	1.00	11.60
4898	N	CYS	B	1110	29.692	8.100	96.517	1.00	10.92
4900	CA	CYS	B	1110	29.008	9.135	97.252	1.00	11.36
4902	CB	CYS	B	1110	29.373	10.502	96.669	1.00	11.52
4905	SG	CYS	B	1110	28.553	11.887	97.471	1.00	13.44
4906	C	CYS	B	1110	27.526	8.854	97.097	1.00	11.23
4907	O	CYS	B	1110	27.074	8.525	95.999	1.00	12.59
4908	N	SER	B	1121	26.786	8.984	98.176	1.00	11.62
4910	CA	SER	B	1121	25.355	8.738	98.146	1.00	12.40
4912	CB	SER	B	1121	24.909	7.880	99.329	1.00	13.35
4915	OG	SER	B	1121	25.244	8.454	100.556	1.00	16.39
4917	C	SER	B	1121	24.533	10.000	98.102	1.00	12.99
4918	O	SER	B	1121	23.396	9.979	97.620	1.00	13.14
4919	N	LYS	B	1132	25.073	11.089	98.632	1.00	12.21
4921	CA	LYS	B	1132	24.354	12.339	98.727	1.00	11.85
4923	CB	LYS	B	1132	23.177	12.234	99.679	1.00	14.07
4926	CG	LYS	B	1132	23.524	11.993	101.102	1.00	16.04
4929	CD	LYS	B	1132	22.268	11.758	101.936	1.00	22.21
4932	CE	LYS	B	1132	22.298	12.578	103.200	1.00	25.39
4935	NZ	LYS	B	1132	21.136	12.292	104.118	1.00	28.97
4939	C	LYS	B	1132	25.318	13.400	99.200	1.00	10.85
4940	O	LYS	B	1132	26.452	13.103	99.578	1.00	9.67
4941	N	TYR	B	1143	24.881	14.644	99.141	1.00	9.74
4943	CA	TYR	B	1143	25.632	15.729	99.717	1.00	9.20
4945	CB	TYR	B	1143	26.498	16.460	98.688	1.00	9.03
4948	CG	TYR	B	1143	25.722	17.150	97.586	1.00	9.02
4949	CD1	TYR	B	1143	25.374	18.469	97.703	1.00	9.78
4951	CE1	TYR	B	1143	24.658	19.115	96.724	1.00	11.36
4953	CZ	TYR	B	1143	24.290	18.412	95.609	1.00	12.32
4954	OH	TYR	B	1143	23.582	19.066	94.611	1.00	11.27
4956	CE2	TYR	B	1143	24.630	17.087	95.464	1.00	10.92
4958	CD2	TYR	B	1143	25.357	16.463	96.441	1.00	10.80
4960	C	TYR	B	1143	24.631	16.673	100.355	1.00	9.78
4961	O	TYR	B	1143	23.429	16.669	100.019	1.00	10.01

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
4962	N	THR	B	1154	25.137	17.493	101.263	1.00	9.47
4964	CA	THR	B	1154	24.338	18.448	102.013	1.00	10.15
4966	CB	THR	B	1154	24.358	18.026	103.476	1.00	11.73
4968	OG1	THR	B	1154	23.731	16.745	103.599	1.00	13.04
4970	CG2	THR	B	1154	23.525	18.954	104.329	1.00	12.40
4974	C	THR	B	1154	24.947	19.830	101.870	1.00	10.79
4975	O	THR	B	1154	26.155	20.007	102.061	1.00	10.14
4976	N	GLU	B	1165	24.113	20.798	101.525	1.00	9.82
4978	CA	GLU	B	1165	24.519	22.180	101.481	1.00	10.23
4980	CB	GLU	B	1165	23.907	22.873	100.274	1.00	11.18
4983	CG	GLU	B	1165	24.367	22.294	98.971	1.00	15.71
4986	CD	GLU	B	1165	23.742	22.967	97.767	1.00	22.02
4987	OE1	GLU	B	1165	23.888	24.203	97.601	1.00	27.03
4988	OE2	GLU	B	1165	23.108	22.248	96.977	1.00	23.03
4989	C	GLU	B	1165	24.032	22.852	102.731	1.00	10.08
4990	O	GLU	B	1165	22.843	22.805	103.059	1.00	11.84
4991	N	LEU	B	1176	24.931	23.519	103.430	1.00	9.65
4993	CA	LEU	B	1176	24.555	24.196	104.650	1.00	9.76
4995	CB	LEU	B	1176	25.770	24.415	105.529	1.00	10.35
4998	CG	LEU	B	1176	26.404	23.137	106.050	1.00	12.53
5000	CD1	LEU	B	1176	27.481	23.557	107.064	1.00	13.35
5004	CD2	LEU	B	1176	25.441	22.136	106.633	1.00	16.89
5008	C	LEU	B	1176	23.927	25.550	104.325	1.00	10.33
5009	O	LEU	B	1176	24.167	26.124	103.261	1.00	10.92
5010	N	PRO	B	1187	23.147	26.085	105.254	1.00	10.89
5011	CA	PRO	B	1187	22.458	27.352	105.014	1.00	11.46
5013	CB	PRO	B	1187	21.554	27.492	106.216	1.00	11.62
5016	CG	PRO	B	1187	22.188	26.672	107.286	1.00	13.14
5019	CD	PRO	B	1187	22.914	25.585	106.616	1.00	12.06
5022	C	PRO	B	1187	23.438	28.504	104.909	1.00	10.68
5023	O	PRO	B	1187	24.467	28.589	105.586	1.00	10.88
5024	N	TYR	B	1198	23.103	29.435	104.048	1.00	10.04
5026	CA	TYR	B	1198	23.979	30.534	103.756	1.00	9.17
5028	CB	TYR	B	1198	23.325	31.469	102.737	1.00	9.53
5031	CG	TYR	B	1198	24.209	32.609	102.374	1.00	7.93
5032	CD1	TYR	B	1198	25.113	32.514	101.332	1.00	8.54
5034	CE1	TYR	B	1198	25.956	33.550	101.045	1.00	8.85
5036	CZ	TYR	B	1198	25.908	34.717	101.765	1.00	8.67
5037	OH	TYR	B	1198	26.797	35.740	101.450	1.00	11.29
5039	CE2	TYR	B	1198	25.040	34.834	102.809	1.00	8.95
5041	CD2	TYR	B	1198	24.189	33.792	103.102	1.00	8.19
5043	C	TYR	B	1198	24.386	31.373	104.975	1.00	9.00
5044	O	TYR	B	1198	23.564	31.914	105.701	1.00	9.23
5045	N	GLY	B	12019	25.694	31.503	105.137	1.00	9.56
5047	CA	GLY	B	12019	26.285	32.366	106.112	1.00	10.15
5050	C	GLY	B	12019	26.228	31.973	1Q7.550	1.00	11.00
5051	O	GLY	B	12019	26.550	32.826	108.366	1.00	12.83
5052	N	ARG	B	1210	25.939	30.723	107.884	1.00	10.72
5054	CA	ARG	B	1210	25.665	30.371	109.273	1.00	11.15
5056	CB	ARG	B	1210	24.384	29.579	109.457	1.00	12.58
5059	CG	ARG	B	1210	23.151	30.424	109.170	1.00	15.83

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5062	CD	ARG	B	1210	22.612	31.062	110.488	1.00	20.35
5065	NE	ARG	B	1210	21.987	30.006	111.303	1.00	26.34
5067	CZ	ARG	B	1210	21.907	29.941	112.624	1.00	26.96
5068	NH1	ARG	B	1210	22.430	30.880	113.409	1.00	30.93
5071	NH2	ARG	B	1210	21.280	28.901	113.164	1.00	28.58
5074	C	ARG	B	1210	26.879	29.641	109.820	1.00	10.93
5075	O	ARG	B	1210	27.060	28.455	109.663	1.00	11.09
5076	N	GLU	B	1221	27.645	30.376	110.596	1.00	10.69
5078	CA	GLU	B	1221	28.952	29.897	111.020	1.00	10.41
5080	CB	GLU	B	1221	29.917	30.998	111.441	1.00	9.85
5083	CG	GLU	B	1221	30.465	31.810	110.294	1.00	10.85
5086	CD	GLU	B	1221	31.599	32.716	110.697	1.00	11.35
5087	OE1	GLU	B	1221	32.768	32.278	110.775	1.00	11.61
5088	OE2	GLU	B	1221	31.276	33.892	110.906	1.00	13.37
5089	C	GLU	B	1221	28.715	28.927	112.150	1.00	10.45
5090	O	GLU	B	1221	29.513	28.017	112.323	1.00	10.51
5091	N	ASP	B	1232	27.610	29.080	112.893	1.00	10.44
5093	CA	ASP	B	1232	27.278	28.115	113.952	1.00	10.75
5095	CB	ASP	B	1232	26.162	28.626	114.884	1.00	11.31
5098	CG	ASP	B	1232	24.956	29.190	114.135	1.00	14.84
5099	OD1	ASP	B	1232	23.952	29.544	114.817	1.00	20.72
5100	OD2	ASP	B	1232	24.882	29.336	112.882	1.00	14.73
5101	C	ASP	B	1232	26.933	26.751	113.351	1.00	10.27
5102	O	ASP	B	1232	27.321	25.710	113.883	1.00	10.55
5103	N	VAL	B	1243	26.208	26.752	112.232	1.00	9.28
5105	CA	VAL	B	1243	25.859	25.509	111.557	1.00	9.51
5107	CB	VAL	B	1243	24.762	25.693	110.510	1.00	9.52
5109	CG1	VAL	B	1243	24.458	24.400	109.819	1.00	10.41
5113	CG2	VAL	B	1243	23.510	26.282	111.175	1.00	10.94
5117	C	VAL	B	1243	27.113	24.878	110.957	1.00	8.40
5118	O	VAL	B	1243	27.284	23.673	110.990	1.00	9.46
5119	N	LEU	B	1254	28.010	25.707	110.453	1.00	8.87
5121	CA	LEU	B	1254	29.261	25.200	109.909	1.00	8.13
5123	CB	LEU	B	1254	30.013	26.319	109.209	1.00	8.65
5126	CG	LEU	B	1254	31.356	25.908	108.620	1.00	7.69
5128	CD1	LEU	B	1254	31.221	24.784	107.616	1.00	8.06
5132	CD2	LEU	B	1254	32.010	27.077	107.992	1.00	8.99
5136	C	LEU	B	1254	30.112	24.551	111.008	1.00	8.15
5137	O	LEU	B	1254	30.668	23.498	110.824	1.00	7.43
5138	N	LYS	B	1265	29.993	25.033	112.224	1.00	9.04
5140	CA	LYS	B	1265	30.818	24.615	113.360	1.00	8.87
5142	CB	LYS	B	1265	30.698	25.573	114.545	1.00	8.48
5145	CG	LYS	B	1265	31.720	25.344	115.619	1.00	9.52
5148	CD	LYS	B	1265	31.299	25.927	116.941	1.00	10.52
5151	CE	LYS	B	1265	32.310	25.640	118.040	1.00	12.18
5154	NZ	LYS	B	1265	31.891	26.221	119.337	1.00	13.54
5158	C	LYS	B	1265	30.296	23.257	113.771	1.00	9.93
5159	O	LYS	B	1265	31.044	22.312	113.958	1.00	8.70
5160	N	GLU	B	1276	28.999	23.069	113.637	1.00	9.98
5162	CA	GLU	B	1276	28.343	21.873	114.104	1.00	10.72
5164	CB	GLU	B	1276	26.815	22.038	114.188	1.00	11.00

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5167	CG	GLU	B	1276	26.133	20.796	114.744	1.00	14.85
5170	CD	GLU	B	1276	24.633	20.983	114.889	1.00	22.12
5171	OE1	GLU	B	1276	23.873	20.276	114.198	1.00	30.96
5172	OE2	GLU	B	1276	24.216	21.834	115.698	1.00	30.51
5173	C	GLU	B	1276	28.675	20.790	113.087	1.00	9.86
5174	O	GLU	B	1276	28.946	19.628	113.434	1.00	9.90
5175	N	ALA	B	1287	28.676	21.150	111.803	1.00	9.24
5177	CA	ALA	B	1287	29.002	20.187	110.767	1.00	8.77
5179	CB	ALA	B	1287	28.716	20.776	109.392	1.00	9.81
5183	C	ALA	B	1287	30.463	19.724	110.862	1.00	8.18
5184	O	ALA	B	1287	30.778	18.546	110.695	1.00	8.99
5185	N	VAL	B	1298	31.357	20.670	111.061	1.00	8.13
5187	CA	VAL	B	1298	32.752	20.307	111.207	1.00	8.78
5189	CB	VAL	B	1298	33.654	21.544	111.241	1.00	8.18
5191	CG1	VAL	B	1298	35.086	21.141	111.491	1.00	10.14
5195	CG2	VAL	B	1298	33.537	22.343	109.925	1.00	9.95
5199	C	VAL	B	1298	32.962	19.420	112.439	1.00	9.42
5200	O	VAL	B	1298	33.706	18.455	112.382	1.00	10.59
5201	N	ALA	B	13029	32.279	19.715	113.535	1.00	9.53
5203	CA	ALA	B	13029	32.446	18.941	114.773	1.00	10.31
5205	CB	ALA	B	13029	31.743	19.666	115.935	1.00	10.22
5209	C	ALA	B	13029	31.884	17.520	114.660	1.00	11.48
5210	O	ALA	B	13029	32.446	16.565	115.195	1.00	13.85
5211	N	ASN	B	1310	30.744	17.402	113.974	1.00	11.81
5213	CA	ASN	B	1310	29.947	16.167	113.977	1.00	12.74
5215	CB	ASN	B	1310	28.507	16.459	114.379	1.00	13.40
5218	CG	ASN	B	1310	28.391	16.955	115.795	1.00	14.96
5219	OD1	ASN	B	1310	29.236	16.647	116.619	1.00	20.90
5220	ND2	ASN	B	1310	27.359	17.743	116.082	1.00	19.85
5223	C	ASN	B	1310	29.909	15.357	112.699	1.00	13.26
5224	O	ASN	B	1310	29.599	14.158	112.741	1.00	15.74
5225	N	LYS	B	1321	30.181	15.994	111.562	1.00	11.33
5227	CA	LYS	B	1321	30.092	15.320	110.272	1.00	10.96
5229	CB	LYS	B	1321	29.182	16.101	109.323	1.00	11.23
5232	CG	LYS	B	1321	27.821	16.322	109.878	1.00	14.86
5235	CD	LYS	B	1321	27.083	14.999	110.018	1.00	19.95
5238	CE	LYS	B	1321	25.624	15.220	110.354	1.00	22.43
5241	NZ	LYS	B	1321	24.842	13.943	110.245	1.00	25.65
5245	C	LYS	B	1321	31.455	15.063	109.645	1.00	10.68
5246	O	LYS	B	1321	31.714	13.963	109.163	1.00	11.64
5247	N	GLY	B	1332	32.325	16.065	109.638	1.00	9.74
5249	CA	GLY	B	1332	33.635	15.942	109.049	1.00	9.35
5252	C	GLY	B	1332	34.040	17.241	108.387	1.00	8.28
5253	O	GLY	B	1332	33.356	18.245	108.521	1.00	8.75
5254	N	PRO	B	1343	35.169	17.223	107.692	1.00	7.92
5255	CA	PRO	B	1343	35.584	18.380	106.903	1.00	7.00
5257	CB	PRO	B	1343	36.828	17.879	106.194	1.00	7.70
5260	CG	PRO	B	1343	37.360	16.860	107.148	1.00	8.79
5263	CD	PRO	B	1343	36.160	16.151	107.625	1.00	8.19
5266	C	PRO	B	1343	34.508	18.799	105.908	1.00	7.17
5267	O	PRO	B	1343	33.807	17.955	105.352	1.00	8.23

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5268	N	VAL	B	1354	34.416	20.100	105.715	1.00	6.17
5270	CA	VAL	B	1354	33.385	20.695	104.894	1.00	6.28
5272	CB	VAL	B	1354	32.455	21.573	105.771	1.00	6.46
5274	CG1	VAL	B	1354	31.419	22.302	104.956	1.00	7.39
5278	CG2	VAL	B	1354	31.792	20.716	106.866	1.00	6.98
5282	C	VAL	B	1354	34.005	21.518	103.777	1.00	6.20
5283	O	VAL	B	1354	34.898	22.335	103.990	1.00	7.03
5284	N	SER	B	1365	33.510	21.296	102.580	1.00	6.73
5286	CA	SER	B	1365	33.946	22.080	101.443	1.00	6.36
5288	CB	SER	B	1365	33.485	21.421	100.151	1.00	6.23
5291	OG	SER	B	1365	34.087	20.176	99.924	1.00	8.76
5293	C	SER	B	1365	33.317	23.450	101.509	1.00	6.66
5294	O	SER	B	1365	32.136	23.584	101.749	1.00	7.48
5295	N	VAL	B	1366	34.114	24.483	101.314	1.00	6.15
5297	CA	VAL	B	1376	33.587	25.844	101.358	1.00	6.50
5299	CB	VAL	B	1376	33.878	26.552	102.725	1.00	6.83
5301	CG1	VAL	B	1376	33.245	25.821	103.877	1.00	8.00
5305	CG2	VAL	B	1376	35.362	26.671	102.940	1.00	8.64
5309	C	VAL	B	1376	34.273	26.650	100.275	1.00	7.02
5310	O	VAL	B	1376	35.319	26.276	99.730	1.00	7.34
5311	N	GLY	B	1387	33.650	27.763	99.944	1.00	7.52
5313	CA	GLY	B	1387	34.285	28.757	99.114	1.00	7.15
5316	C	GLY	B	1387	34.701	29.952	99.928	1.00	9.04
5317	O	GLY	B	1387	34.040	30.318	100.896	1.00	9.03
5318	N	VAL	B	1398	35.799	30.577	99.520	1.00	7.47
5320	CA	VAL	B	1398	36.242	31.787	100.162	1.00	9.05
5322	CB	VAL	B	1398	37.464	31.583	101.093	1.00	9.17
5324	CG1	VAL	B	1398	37.077	30.671	102.220	1.00	9.47
5328	CG2	VAL	B	1398	38.696	31.043	100.357	1.00	8.11
5332	C	VAL	B	1398	36.573	32.819	99.150	1.00	8.77
5333	O	VAL	B	1398	36.881	32.499	98.004	1.00	9.48
5334	N	ASP	B	14039	36.518	34.073	99.567	1.00	9.97
5336	CA	ASP	B	14039	37.026	35.178	98.760	1.00	10.54
5338	CB	ASP	B	14039	36.393	36.476	99.249	1.00	10.83
5341	CG	ASP	B	14039	36.949	37.700	98.570	1.00	14.11
5342	OD1	ASP	B	14039	37.762	37.557	97.637	1.00	13.49
5343	OD2	ASP	B	14039	36.600	38.846	98.903	1.00	15.62
5344	C	ASP	B	14039	38.535	35.217	98.949	1.00	11.52
5345	O	ASP	B	14039	39.022	35.614	100.003	1.00	11.69
5346	N	ALA	B	1410	39.264	34.747	97.939	1.00	12.09
5348	CA	ALA	B	1410	40.721	34.706	97.981	1.00	12.78
5350	CB	ALA	B	1410	41.207	33.297	97.667	1.00	13.40
5354	C	ALA	B	1410	41.319	35.671	96.985	1.00	13.87
5355	O	ALA	B	1410	42.426	35.467	96.505	1.00	14.51
5356	N	LYS	B	1421	40.737	36.837	96.854	1.00	14.99
5358	CA	LYS	B	1421	41.063	37.713	95.713	1.00	16.31
5360	CB	LYS	B	1421	39.836	38.370	95.093	1.00	17.07
5363	CG	LYS	B	1421	38.989	37.436	94.228	1.00	20.76
5366	CD	LYS	B	1421	38.135	38.210	93.228	1.00	24.19
5369	CE	LYS	B	1421	36.825	38.589	93.829	1.00	26.69
5372	NZ	LYS	B	1421	35.976	37.446	94.259	1.00	26.99

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5376	C	LYS	B	142~~1~~	42.046	38.762	96.187	1.00	16.96
5377	O	LYS	B	142~~1~~	42.658	39.480	95.379	1.00	20.53
5378	N	HIS	B	143~~2~~	42.287	38.815	97.477	1.00	14.88
5380	CA	HIS	B	143~~2~~	43.092	39.890	98.036	1.00	14.46
5382	CB	HIS	B	143~~2~~	42.464	40.356	99.343	1.00	15.50
5385	CG	HIS	B	143~~2~~	41.007	40.603	99.192	1.00	15.75
5386	ND1	HIS	B	143~~2~~	40.506	41.776	98.672	1.00	18.10
5388	CE1	HIS	B	143~~2~~	39.192	41.686	98.584	1.00	20.19
5390	NE2	HIS	B	143~~2~~	38.830	40.484	98.991	1.00	18.79
5392	CD2	HIS	B	143~~2~~	39.944	39.786	99.367	1.00	18.55
5394	C	HIS	B	143~~2~~	44.539	39.455	98.175	1.00	13.69
5395	O	HIS	B	143~~2~~	44.845	38.313	98.455	1.00	12.93
5396	N	PRO	B	144~~3~~	45.466	40.356	97.907	1.00	13.23
5397	CA	PRO	B	144~~3~~	46.879	39.998	97.972	1.00	12.65
5399	CB	PRO	B	144~~3~~	47.582	41.344	97.740	1.00	13.88
5402	CG	PRO	B	144~~3~~	46.509	42.387	97.847	1.00	15.37
5405	CD	PRO	B	144~~3~~	45.257	41.746	97.469	1.00	13.32
5408	C	PRO	B	144~~3~~	47.254	39.364	99.319	1.00	11.62
5409	O	PRO	B	144~~3~~	48.103	38.501	99.347	1.00	12.09
5410	N	SER	B	145~~4~~	46.608	39.785	100.402	1.00	11.24
5412	CA	SER	B	145~~4~~	46.877	39.236	101.726	1.00	10.46
5414	CB	SER	B	145~~4~~	45.997	39.909	102.761	1.00	11.01
5417	OG	SER	B	145~~4~~	44.640	39.765	102.420	1.00	11.77
5419	C	SER	B	145~~4~~	46.692	37.713	101.784	1.00	10.39
5420	O	SER	B	145~~4~~	47.364	37.050	102.541	1.00	10.75
5421	N	PHE	B	146~~5~~	45.758	37.185	101.009	1.00	9.85
5423	CA	PHE	B	146~~5~~	45.532	35.754	100.990	1.00	9.97
5425	CB	PHE	B	146~~5~~	44.247	35.432	100.264	1.00	9.49
5428	CG	PHE	B	146~~5~~	43.818	34.011	100.413	1.00	9.57
5429	CD1	PHE	B	146~~5~~	44.314	33.032	99.579	1.00	10.99
5431	CE1	PHE	B	146~~5~~	43.923	31.728	99.749	1.00	12.44
5433	CZ	PHE	B	146~~5~~	43.027	31.413	100.721	1.00	10.41
5435	CE2	PHE	B	146~~5~~	42.524	32.372	101.545	1.00	11.02
5437	CD2	PHE	B	146~~5~~	42.914	33.659	101.397	1.00	12.00
5439	C	PHE	B	146~~5~~	46.742	35.055	100.370	1.00	10.60
5440	O	PHE	B	146~~5~~	47.263	34.087	100.898	1.00	10.44
5441	N	PHE	B	147~~6~~	47.214	35.574	99.247	1.00	11.47
5443	CA	PHE	B	147~~6~~	48.356	34.992	98.574	1.00	11.39
5445	CB	PHE	B	147~~6~~	48.621	35.696	97.249	1.00	11.64
5448	CG	PHE	B	147~~6~~	47.608	35.399	96.200	1.00	10.84
5449	CD1	PHE	B	147~~6~~	47.849	34.451	95.228	1.00	10.86
5451	CE1	PHE	B	147~~6~~	46.904	34.176	94.274	1.00	10.08
5453	CZ	PHE	B	147~~6~~	45.706	34.820	94.301	1.00	11.86
5455	CE2	PHE	B	147~~6~~	45.466	35.760	95.250	1.00	12.59
5457	CD2	PHE	B	147~~6~~	46.387	36.033	96.201	1.00	12.51
5459	C	PHE	B	147~~6~~	49.601	35.107	99.427	1.00	11.66
5460	O	PHE	B	147~~6~~	·50.477	34.242	99.354	1.00	13.04
5461	N	LEU	B	148~~7~~	49.688	36.178	100.195	1.00	10.78
5463	CA	LEU	B	148~~7~~	50.870	36.472	100.987	1.00	11.88
5465	CB	LEU	B	148~~7~~	51.093	37.983	101.057	1.00	12.57
5468	CG	LEU	B	148~~7~~	51.343	38.603	99.700·	1.00	14.42

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5470	CD1	LEU	B	148~~7~~	51.317	40.125	99.797	1.00	16.61
5474	CD2	LEU	B	148~~7~~	52.648	38.114	99.127	1.00	15.72
5478	C	LEU	B	148~~7~~	50.809	35.909	102.388	1.00	11.97
5479	O	LEU	B	148~~7~~	51.755	36.043	103.150	1.00	13.07
5480	N	TYR	B	149~~8~~	49.691	35.285	102.744	1.00	11.31
5482	CA	TYR	B	149~~8~~	49.543	34.719	104.080	1.00	10.51
5484	CB	TYR	B	149~~8~~	48.211	34.014	104.166	1.00	9.45
5487	CG	TYR	B	149~~8~~	48.024	33.227	105.423	1.00	8.58
5488	CD1	TYR	B	149~~8~~	48.279	31.870	105.448	1.00	7.97
5490	CE1	TYR	B	149~~8~~	48.125	31.145	106.592	1.00	9.23
5492	CZ	TYR	B	149~~8~~	47.666	31.746	107.738	1.00	8.37
5493	OH	TYR	B	149~~8~~	47.462	30.982	108.828	1.00	9.21
5495	CE2	TYR	B	149~~8~~	47.377	33.094	107.741	1.00	8.94
5497	CD2	TYR	B	149~~8~~	47.587	33.824	106.590	1.00	8.72
5499	C	TYR	B	149~~8~~	50.631	33.742	104.475	1.00	11.02
5500	O	TYR	B	149~~8~~	50.974	32.838	103.710	1.00	11.67
5501	N	ARG	B	1504~~9~~	51.128	33.914	105.695	1.00	12.05
5503	CA	ARG	B	1504~~9~~	52.128	33.018	106.229	1.00	13.10
5505	CB	ARG	B	1504~~9~~	53.404	33.808	106.523	1.00	13.66
5508	CG	ARG	B	1504~~9~~	54.060	34.285	105.259	1.00	16.66
5511	CD	ARG	B	1504~~9~~	54.488	33.128	104.369	1.00	23.21
5514	NE	ARG	B	1504~~9~~	55.714	32.515	104.877	1.00	27.93
5516	CZ	ARG	B	1504~~9~~	56.329	31.476	104.330	1.00	34.05
5517	NH1	ARG	B	1504~~9~~	57.473	31.030	104.846	1.00	36.85
5520	NH2	ARG	B	1504~~9~~	55.799	30.871	103.274	1.00	36.34
5523	C	ARG	B	1504~~9~~	51.725	32.280	107.469	1.00	13.08
5524	O	ARG	B	1504~~9~~	52.000	31.086	107.595	1.00	13.40
5525	N	SER	B	151~~0~~	51.115	32.975	108.416	1.00	12.69
5527	CA	SER	B	151~~0~~	50.807	32.340	109.684	1.00	13.15
5529	CB	SER	B	151~~0~~	52.087	32.213	110.514	1.00	14.45
5532	OG	SER	B	151~~0~~	52.525	33.494	110.887	1.00	17.66
5534	C	SER	B	151~~0~~	49.794	33.132	110.463	1.00	12.22
5535	O	SER	B	151~~0~~	49.538	34.307	110.166	1.00	13.35
5536	N	GLY	B	152~~1~~	49.212	32.479	111.462	1.00	11.61
5538	CA	GLY	B	152~~1~~	48.263	33.130	112.342	1.00	11.64
5541	C	GLY	B	152~~1~~	46.856	33.143	111.797	1.00	11.53
5542	O	GLY	B	152~~1~~	46.522	32.417	110.857	1.00	12.06
5543	N	VAL	B	153~~2~~	46.021	33.989	112.380	1.00	10.63
5545	CA	VAL	B	153~~2~~	44.619	34.030	111.976	1.00	10.56
5547	CB	VAL	B	153~~2~~	43.672	34.242	113.135	1.00	11.08
5549	CG1	VAL	B	153~~2~~	42.225	34.346	112.641	1.00	10.84
5553	CG2	VAL	B	153~~2~~	43.822	33.132	114.163	1.00	11.34
5557	C	VAL	B	153~~2~~	44.450	35.094	110.923	1.00	11.19
5558	O	VAL	B	153~~2~~	44.689	36.288	111.161	1.00	13.43
5559	N	TYR	B	154~~3~~	44.037	34.663	109.747	1.00	9.55
5561	CA	TYR	B	154~~3~~	43.839	35.570	108.645	1.00	9.45
5563	CB	TYR	B	154~~3~~	43.704	34.759	107.358	1.00	8.66
5566	CG	TYR	B	154~~3~~	43.493	35.564	106.104	1.00	9.70
5567	CD1	TYR	B	154~~3~~	44.526	36.256	105.541	1.00	8.14
5569	CE1	TYR	B	154~~3~~	44.361	36.975	104.395	1.00	8.81
5571	CZ	TYR	B	154~~3~~	43.149	36.989	103.775	1.00	8.19

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5572	OH	TYR	B	1543	42.961	37.724	102.626	1.00	9.19
5574	CE2	TYR	B	1543	42.091	36.314	104.333	1.00	8.29
5576	CD2	TYR	B	1543	42.276	35.594	105.476	1.00	8.68
5578	C	TYR	B	1543	42.595	36.397	108.795	1.00	9.48
5579	O	TYR	B	1543	41.493	35.882	108.941	1.00	9.95
5580	N	TYR	B	1554	42.761	37.702	108.614	1.00	10.50
5582	CA	TYR	B	1554	41.625	38.614	108.679	1.00	11.82
5584	CB	TYR	B	1554	41.266	39.027	110.118	1.00	12.51
5587	CG	TYR	B	1554	40.133	40.009	110.202	1.00	14.71
5588	CD1	TYR	B	1554	38.830	39.598	110.413	1.00	16.28
5590	CE1	TYR	B	1554	37.794	40.507	110.488	1.00	18.67
5592	CZ	TYR	B	1554	38.064	41.839	110.395	1.00	21.95
5593	OH	TYR	B	1554	37.008	42.742	110.468	1.00	24.21
5595	CE2	TYR	B	1554	39.353	42.273	110.213	1.00	21.50
5597	CD2	TYR	B	1554	40.384	41.356	110.127	1.00	19.87
5599	C	TYR	B	1554	41.940	39.761	107.719	1.00	12.04
5600	O	TYR	B	1554	42.983	40.419	107.805	1.00	13.44
5601	N	GLU	B	1565	41.092	39.938	106.732	1.00	11.56
5603	CA	GLU	B	1565	41.306	40.933	105.733	1.00	12.76
5605	CB	GLU	B	1565	41.418	40.198	104.405	1.00	13.09
5608	CG	GLU	B	1565	41.430	41.087	103.182	1.00	14.67
5611	CD	GLU	B	1565	42.419	42.227	103.270	1.00	17.56
5612	OE1	GLU	B	1565	41.941	43.387	103.365	1.00	18.67
5613	OE2	GLU	B	1565	43.663	41.996	103.238	1.00	17.06
5614	C	GLU	B	1565	40.131	41.880	105.702	1.00	13.27
5615	O	GLU	B	1565	39.052	41.505	105.253	1.00	12.29
5616	N	PRO	B	1576	40.323	43.106	106.169	1.00	14.16
5617	CA	PRO	B	1576	39.229	44.083	106.177	1.00	15.60
5619	CB	PRO	B	1576	39.927	45.383	106.589	1.00	15.91
5622	CG	PRO	B	1576	41.119	44.942	107.424	1.00	15.73
5625	CD	PRO	B	1576	41.541	43.619	106.819	1.00	15.55
5628	C	PRO	B	1576	38.506	44.269	104.833	1.00	15.84
5629	O	PRO	B	1576	37.341	44.642	104.829	1.00	17.36
5630	N	SER	B	1587	39.183	44.036	103.713	1.00	15.22
5632	CA	SER	B	1587	38.588	44.209	102.390	1.00	16.32
5634	CB	SER	B	1587	39.673	44.606	101.389	1.00	17.36
5637	OG	SER	B	1587	40.076	45.965	101.564	1.00	20.95
5639	C	SER	B	1587	37.858	42.953	101.888	1.00·15.52	
5640	O	SER	B	1587	37.275	42.957	100.806	1.00	15.55
5641	N	CYS	B	1598	37.903	41.874	102.654	1.00	15.43
5643	CA	CYS	B	1598	37.241	40.643	102.240	1.00	15.62
5645	CB	CYS	B	1598	37.495	39.505	103.227	1.00	15.41
5648	SG	CYS	B	1598	38.336	38.143	102.397	1.00	20.02
5649	C	CYS	B	1598	35.747	40.829	102.095	1.00	16.39
5650	O	CYS	B	1598	35.158	41.671	102.743	1.00	17.26
5651	N	THR	B	16059	35.147	40.023	101.236	1.00	16.17
5653	CA	THR	B	16059	33.710	40.088	101.033	1.00	16.60
5655	CB	THR	B	16059	33.390	40.690	99.679	1.00	17.48
5657	OG1	THR	B	16059	33.791	39.783	98.630	1.00	18.28
5659	CG2	THR	B	16059	34.203	41.973	99.470	1.00	19.79
5663	C	THR	B	16059	33.153	38.704	101.090	1.00	16.64

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5664	O	THR	B	160~~59~~	33.886	37.757	101.277	1.00	14.66
5665	N	GLN	B	161~~0~~	31.841	38.556	100.937	1.00	16.68
5667	CA	GLN	B	161~~0~~	31.359	37.188	100.913	1.00	18.21
5669	CB	GLN	B	161~~0~~	30.220	36.852	101.886	1.00	19.79
5672	CG	GLN	B	161~~0~~	29.445	37.876	102.466	1.00	20.69
5675	CD	GLN	B	161~~0~~	30.197	38.882	103.330	1.00	17.61
5676	OE1	GLN	B	161~~0~~	30.912	38.573	104.303	1.00	22.35
5677	NE2	GLN	B	161~~0~~	29.999	40.105	102.985	1.00	13.41
5680	C	GLN	B	161~~0~~	31.098	36.680	99.513	1.00	18.73
5681	O	GLN	B	161~~0~~	30.415	35.662	99.355	1.00	20.53
5682	N	ASN	B	162~~1~~	31.712	37.315	98.521	1.00	18.63
5684	CA	ASN	B	162~~1~~	31.624	36.834	97.142	1.00	19.19
5686	CB	ASN	B	162~~1~~	31.425	37.981	96.186	1.00	20.60
5689	CG	ASN	B	162~~1~~	29.934	38.268	95.967	1.00	21.63
5690	OD1	ASN	B	162~~1~~	29.153	37.387	95.506	1.00	26.69
5691	ND2	ASN	B	162~~1~~	29.521	39.442	96.343	1.00	24.94
5694	C	ASN	B	162~~1~~	32.829	35.916	96.889	1.00	17.43
5695	O	ASN	B	162~~1~~	33.991	36.354	96.749	1.00	19.14
5696	N	VAL	B	163~~2~~	32.529	34.628	96.932	1.00	14.34
5698	CA	VAL	B	163~~2~~	33.564	33.615	96.996	1.00	12.85
5700	CB	VAL	B	163~~2~~	33.121	32.387	97.834	1.00	12.66
5702	CG1	VAL	B	163~~2~~	32.704	32.826	99.240	1.00	13.58
5706	CG2	VAL	B	163~~2~~	32.015	31.638	97.180	1.00	14.06
5710	C	VAL	B	163~~2~~	34.054	33.163	95.633	1.00	11.50
5711	O	VAL	B	163~~2~~	33.267	33.099	94.671	1.00	12.03
5712	N	ASN	B	164~~3~~	35.344	32.854	95.537	1.00	10.09
5714	CA	ASN	B	164~~3~~	35.910	32.452	94.256	1.00	10.38
5716	CB	ASN	B	164~~3~~	36.623	33.630	93.587	1.00	11.24
5719	CG	ASN	B	164~~3~~	37.948	33.936	94.216	1.00	13.93
5720	OD1	ASN	B	164~~3~~	38.037	34.064	95.411	1.00	12.67
5721	ND2	ASN	B	164~~3~~	39.012	33.972	93.409	1.00	18.85
5724	C	ASN	B	164~~3~~	36.883	31.330	94.347	1.00	9.44
5725	O	ASN	B	164~~3~~	37.464	30.937	93.337	1.00	12.04
5726	N	HIS	B	165~~4~~	37.093	30.781	95.537	1.00	8.88
5728	CA	HIS	B	165~~4~~	38.139	29.774	95.683	1.00	8.02
5730	CB	HIS	B	165~~4~~	39.384	30.461	96.240	1.00	8.65
5733	CG	HIS	B	165~~4~~	40.550	29.555	96.422	1.00	10.78
5734	ND1	HIS	B	165~~4~~	41.083	28.824	95.382	1.00	15.76
5736	CE1	HIS	B	165~~4~~	42.105	28.112	95.830	1.00	15.67
5738	NE2	HIS	B	165~~4~~	42.270	28.386	97.108	1.00	12.26
5740	CD2	HIS	B	165~~4~~	41.302	29.275	97.507	1.00	12.81
5742	C	HIS	B	165~~4~~	37.690	28.678	96.639	1.00	8.33
5743	O	HIS	B	165~~4~~	37.384	28.941	97.786	1.00	9.64
5744	N	GLY	B	166~~5~~	37.634	27.468	96.148	1.00	7.46
5746	CA	GLY	B	166~~5~~	37.223	26.334	96.935	1.00	7.29
5749	C	GLY	B	166~~5~~	38.328	25.793	97.794	1.00	7.51
5750	O	GLY	B	166~~5~~	39.429	25.578	97.330	1.00	9.21
5751	N	VAL	B	167~~6~~	38.019	25.567	99.064	1.00	7.37
5753	CA	VAL	B	167~~6~~	38.962	25.031	100.054	1.00	6.65
5755	CB	VAL	B	167~~6~~	39.612	26.132	100.887	1.00	6.93
5757	CG1	VAL	B	167~~6~~	40.495	27.016	99.966	1.00	9.91

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5761	CG2	VAL	B	1676	38.556	26.939	101.587	1.00	7.95
5765	C	VAL	B	1676	38.202	24.093	100.971	1.00	6.60
5766	O	VAL	B	1676	37.018	23.823	100.786	1.00	6.50
5767	N	LEU	B	1687	38.900	23.550	101.965	1.00	6.10
5769	CA	LEU	B	1687	38.294	22.550	102.832	1.00	5.61
5771	CB	LEU	B	1687	38.965	21.199	102.588	1.00	6.00
5774	CG	LEU	B	1687	38.386	20.031	103.353	1.00	7.01
5776	CD1	LEU	B	1687	37.010	19.680	102.806	1.00	6.78
5780	CD2	LEU	B	1687	39.311	18.834	103.260	1.00	8.35
5784	C	LEU	B	1687	38.495	22.949	104.279	1.00	6.09
5785	O	LEU	B	1687	39.620	23.139	104.711	1.00	6.83
5786	N	VAL	B	1698	37.405	23.045	105.029	1.00	5.80
5788	CA	VAL	B	1698	37.516	23.346	106.430	1.00	6.41
5790	CB	VAL	B	1698	36.251	24.017	106.967	1.00	6.62
5792	CG1	VAL	B	1698	36.382	24.204	108.459	1.00	6.69
5796	CG2	VAL	B	1698	36.030	25.347	106.282	1.00	8.01
5800	C'	VAL	B	1698	37.725	22.013	107.127	1.00	6.07
5801	O	VAL	B	1698	36.856	21.154	107.098	1.00	7.50
5802	N	VAL	B	17069	38.866	21.868	107.798	1.00	6.18
5804	CA	VAL	B	17069	39.194	20.622	108.477	1.00	6.52
5806	CB	VAL	B	17069	40.532	20.020	107.999	1.00	6.54
5808	CG1	VAL	B	17069	40.450	19.666	106.514	1.00	7.17
5812	CG2	VAL	B	17069	41.680	20.954	108.264	1.00	8.62
5816	C	VAL	B	17069	39.239	20.772	109.965	1.00	7.13
5817	O	VAL	B	17069	39.633	19.833	110.659	1.00	8.39
5818	N	GLY	B	1710	38.838	21.919	110.474	1.00	6.69
5820	CA	GLY	B	1710	38.777	22.104	111.907	1.00	7.58
5823	C	GLY	B	1710	38.482	23.530	112.268	1.00	7.72
5824	O	GLY	B	1710	38.166	24.370	111.426	1.00	7.68
5825	N	TYR	B	1721	38.570	23.814	113.565	1.00	7.68
5827	CA	TYR	B	1721	38.370	25.154	114.064	1.00	7.26
5829	CB	TYR	B	1721	36.888	25.512	114.111	1.00	7.75
5832	CG	TYR	B	1721	36.026	24.639	114.994	1.00	7.71
5833	CD1	TYR	B	1721	36.006	24.803	116.371	1.00	9.26
5835	CE1	TYR	B	1721	35.219	24.048	117.154	1.00	8.67
5837	CZ	TYR	B	1721	34.430	23.091	116.610	1.00	8.96
5838	OH	TYR	B	1721	33.602	22.308	117.380	1.00	9.71
5840	CE2	TYR	B	1721	34.398	22.903	115.248	1.00	10.07
5842	CD2	TYR	B	1721	35.194	23.680	114.446	1.00	7.92
5844	C	TYR	B	1721	39.018	25.224	115.451	1.00	7.92
5845	O	TYR	B	1721	39.287	24.204	116.065	1.00	8.32
5846	N	GLY	B	1732	39.221	26.429	115.953	1.00	9.22
5848	CA	GLY	B	1732	39.844	26.612	117.239	1.00	9.98
5851	C	GLY	B	1732	39.966	28.090	117.494	1.00	11.46
5852	O	GLY	B	1732	39.221	28.906	116.938	1.00	9.65
5853	N	ASP	B	1743	40.891	28.427	118.377	1.00	12.30
5855	CA	ASP	B	1743	41.140	29.786	118.778	1.00	14.56
5857	CB	ASP	B	1743	40.384	30.097	120.055	1.00	14.89
5860	CG	ASP	B	1743	40.640	29.054	121.154	1.00	21.20
5861	OD1	ASP	B	1743	41.804	28.938	121.609	1.00	33.99
5862	OD2	ASP	B	1743	39.759	28.307	121.633	1.00	30.54

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5863	C	ASP	B	1743	42.635	29.920	119.011	1.00	15.12
5864	O	ASP	B	1743	43.322	28.961	119.420	1.00	16.70
5865	N	LEU	B	1754	43.113	31.111	118.691	1.00	15.94
5867	CA	LEU	B	1754	44.498	31.482	118.885	1.00	17.52
5869	CB	LEU	B	1754	45.238	31.552	117.541	1.00	17.42
5872	CG	LEU	B	1754	46.692	32.017	117.658	1.00	19.48
5874	CD1	LEU	B	1754	47.503	31.068	118.496	1.00	21.56
5878	CD2	LEU	B	1754	47.342	32.214	116.290	1.00	20.43
5882	C	LEU	B	1754	44.559	32.817	119.624	1.00	19.18
5883	O	LEU	B	1754	44.303	33.876	119.048	1.00	20.27
5884	N	ASN	B	1765	44.842	32.764	120.918	1.00	23.16
5886	CA	ASN	B	1765	44.989	34.008	121.695	1.00	24.79
5888	CB	ASN	B	1765	46.379	34.566	121.530	1.00	25.89
5891	CG	ASN	B	1765	47.334	33.645	122.178	1.00	27.62
5892	OD1	ASN	B	1765	46.924	32.910	123.060	1.00	32.87
5893	ND2	ASN	B	1765	48.497	33.536	121.755	1.00	30.87
5896	C	ASN	B	1765	43.837	34.985	121.530	1.00	24.96
5897	O	ASN	B	1765	43.987	36.180	121.202	1.00	26.41
5898	N	GLY	B	1776	42.676	34.405	121.806	1.00	25.21
5900	CA	GLY	B	1776	41.387	35.062	121.759	1.00	23.98
5903	C	GLY	B	1776	40.844	35.281	120.355	1.00	23.03
5904	O	GLY	B	1776	39.887	36.038	120.164	1.00	24.16
5905	N	ALA	B	1787	41.471	34.674	119.353	1.00	19.96
5907	CA	ALA	B	1787	41.022	34.887	118.000	1.00	17.59
5909	CB	ALA	B	1787	42.127	35.443	117.148	1.00	17.70
5913	C	ALA	B	1787	40.550	33.567	117.430	1.00	13.89
5914	O	ALA	B	1787	41.357	32.701	117.138	1.00	12.51
5915	N	GLU	B	1798	39.238	33.448	117.242	1.00	12.04
5917	CA	GLU	B	1798	38.643	32.230	116.758	1.00	10.60
5919	CB	GLU	B	1798	37.142	32.246	116.980	1.00	12.11
5922	CG	GLU	B	1798	36.786	32.332	118.460	1.00	15.19
5925	CD	GLU	B	1798	35.312	32.201	118.720	1.00	19.64
5926	OE1	GLU	B	1798	34.924	31.215	119.384	1.00	22.49
5927	OE2	GLU	B	1798	34.557	33.109	118.294	1.00	23.85
5928	C	GLU	B	1798	38.979	32.072	115.290	1.00	9.89
5929	O	GLU	B	1798	39.051	33.055	114.529	1.00	9.14
5930	N	TYR	B	179———180		39.159	30.827	114.881	1.00	8.60
5932	CA	TYR	B	179———180		39.541	30.563	113.504	1.00	8.61
5934	CB	TYR	B	18079	41.088	30.438	113.373	1.00	9.24
5937	CG	TYR	B	18079	41.744	29.268	114.136	1.00	9.54
5938	CD1	TYR	B	18079	41.738	27.984	113.626	1.00	8.66
5940	CE1	TYR	B	18079	42.332	26.893	114.330	1.00	13.71
5942	CZ	TYR	B	18079	43.027	27.102	115.546	1.00	16.98
5943	OH	TYR	B	18079	43.597	26.048	116.253	1.00	22.27
5945	CE2	TYR	B	18079	43.014	28.369	116.092	1.00	15.79
5947	CD2	TYR	B	18079	42.413	29.456	115.380	1.00	12.99
5949	C	TYR	B	18079	38.898	29.291	112.974	1.00	7.75
5950	O	TYR	B	18079	38.476	28.430	113.724	1.00	7.96
5951	N	TRP	B	1810	38.818	29.229	111.638	1.00	7.07
5953	CA	TRP	B	1810	38.552	28.027	110.878	1.00	7.09
5955	CB	TRP	B	1810	37.713	28.364	109.645	1.00	6.52

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
5958	CG	TRP	B	1810	36.353	28.817	109.990	1.00	6.60
5959	CD1	TRP	B	1810	35.843	30.076	109.831	1.00	6.36
5961	NE1	TRP	B	1810	34.534	30.111	110.240	1.00	7.27
5963	CE2	TRP	B	1810	34.174	28.874	110.690	1.00	7.07
5964	CD2	TRP	B	1810	35.291	28.026	110.533	1.00	6.65
5965	CE3	TRP	B	1810	35.179	26.706	110.944	1.00	8.43
5967	CZ3	TRP	B	1810	33.971	26.281	111.484	1.00	7.11
5969	CH2	TRP	B	1810	32.899	27.134	111.603	1.00	8.05
5971	CZ2	TRP	B	1810	32.975	28.429	111.235	1.00	6.73
5973	C	TRP	B	1810	39.889	27.515	110.372	1.00	6.50
5974	O	TRP	B	1810	40.695	28.286	109.884	1.00	6.99
5975	N	LEU	B	1821	40.122	26.220	110.481	1.00	5.89
5977	CA	LEU	B	1821	41.347	25.596	109.970	1.00	6.62
5979	CB	LEU	B	1821	41.769	24.413	110.831	1.00	7.19
5982	CG	LEU	B	1821	43.012	23.658	110.369	1.00	9.61
5984	CD1	LEU	B	1821	44.194	24.571	110.280	1.00	10.31
5988	CD2	LEU	B	1821	43.274	22.508	111.308	1.00	10.51
5992	C	LEU	B	1821	41.073	25.129	108.553	1.00	6.29
5993	O	LEU	B	1821	40.240	24.239	108.353	1.00	6.93
5994	N	VAL	B	1832	41.755	25.745	107.587	1.00	6.45
5996	CA	VAL	B	1832	41.461	25.502	106.180	1.00	7.13
5998	CB	VAL	B	1832	41.122	26.826	105.515	1.00	6.74
6000	CG1	VAL	B	1832	40.953	26.682	104.013	1.00	9.42
6004	CG2	VAL	B	1832	39.868	27.455	106.177	1.00	8.63
6008	C	VAL	B	1832	42.611	24.885	105.434	1.00	6.75
6009	O	VAL	B	1832	43.731	25.390	105.512	1.00	7.21
6010	N	LYS	B	1843	42.320	23.791	104.743	1.00	6.74
6012	CA	LYS	B	1843	43.269	23.118	103.881	1.00	6.51
6014	CB	LYS	B	1843	42.967	21.630	103.809	1.00	6.94
6017	CG	LYS	B	1843	44.015	20.831	103.053	1.00	8.30
6020	CD	LYS	B	1843	43.559	19.421	102.814	1.00	9.04
6023	CE	LYS	B	1843	44.704	18.562	102.306	1.00	8.99
6026	NZ	LYS	B	1843	44.202	17.289	101.712	1.00	11.07
6030	C	LYS	B	1843	43.131	23.728	102.483	1.00	7.54
6031	O	LYS	B	1843	42.067	23.700	101.914	1.00	6.69
6032	N	ASN	B	1854	44.198	24.287	101.964	1.00	7.67
6034	CA	ASN	B	1854	44.210	24.840	100.617	1.00	8.28
6036	CB	ASN	B	1854	44.973	26.163	100.637	1.00	8.39
6039	CG	ASN	B	1854	44.698	27.061	99.448	1.00	9.11
6040	OD1	ASN	B	1854	43.876	26.756	98.600	1.00	11.82
6041	ND2	ASN	B	1854	45.441	28.163	99.367	1.00	11.45
6044	C	ASN	B	1854	44.857	23.821	99.690	1.00	8.32
6045	O	ASN	B	1854	45.294	22.778	100.121	1.00	9.99
6046	N	SER	B	1865	44.867	24.125	98.400	1.00	7.52
6048	CA	SER	B	1865	45.478	23.269	97.397	1.00	7.63
6050	CB	SER	B	1865	44.422	22.693	96.460	1.00	8.31
6053	OG	SER	B	1865	43.592	23.694	95.916	1.00	10.44
6055	C	SER	B	1865	46.508	24.055	96.599	1.00	8.21
6056	O	SER	B	1865	46.619	23.897	95.363	1.00	9.13
6057	N	TRP	B	1876	47.271	24.882	97.308	1.00	7.49
6059	CA	TRP	B	1876	48.358	25.657	96.726	1.00	8.01

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6061	CB	TRP	B	1876	48.211	27.120	97.145	1.00	8.80
6064	CG	TRP	B	1876	47.116	27.865	96.436	1.00	8.97
6065	CD1	TRP	B	1876	46.265	27.392	95.470	1.00	11.08
6067	NE1	TRP	B	1876	45.420	28.394	95.053	1.00	13.79
6069	CE2	TRP	B	1876	45.706	29.534	95.755	1.00	13.15
6070	CD2	TRP	B	1876	46.767	29.234	96.631	1.00	10.02
6071	CE3	TRP	B	1876	47.215	30.237	97.498	1.00	12.13
6073	CZ3	TRP	B	1876	46.639	31.477	97.415	1.00	12.53
6075	CH2	TRP	B	1876	45.610	31.740	96.536	1.00	12.01
6077	CZ2	TRP	B	1876	45.115	30.783	95.705	1.00	14.46
6079	C	TRP	B	1876	49.721	25.099	97.128	1.00	9.54
6080	O	TRP	B	1876	50.727	25.799	97.128	1.00	10.61
6081	N	GLY	B	1887	49.744	23.825	97.486	1.00	9.77
6083	CA	GLY	B	1887	50.979	23.166	97.862	1.00	10.92
6086	C	GLY	B	1887	51.372	23.383	99.292	1.00	12.23
6087	O	GLY	B	1887	50.809	24.218	100.004	1.00	11.00
6088	N	HIS	B	1898	52.382	22.640	99.711	1.00	14.93
6090	CA	HIS	B	1898	52.794	22.664	101.101	1.00	17.52
6092	CB	HIS	B	1898	53.572	21.393	101.459	1.00	19.26
6095	CG	HIS	B	1898	54.838	21.226	100.689	1.00	23.21
6096	ND1	HIS	B	1898	55.016	20.221	99.766	1.00	30.10
6098	CE1	HIS	B	1898	56.228	20.315	99.250	1.00	29.61
6100	NE2	HIS	B	1898	56.840	21.345	99.804	1.00	30.15
6102	CD2	HIS	B	1898	55.991	21.931	100.710	1.00	27.77
6104	C	HIS	B	1898	53.567	23.901	101.498	1.00	18.56
6105	O	HIS	B	1898	53.820	24.081	102.692	1.00	20.82
6106	N	ASN	B	19089	53.961	24.742	100.544	1.00	18.78
6108	CA	ASN	B	19089	54.701	25.967	100.867	1.00	19.85
6110	CB	ASN	B	19089	55.752	26.306	99.802	1.00	20.99
6113	CG	ASN	B	19089	56.821	25.234	99.679	1.00	24.70
6114	OD1	ASN	B	19089	57.206	24.849	98.572	1.00	30.00
6115	ND2	ASN	B	19089	57.288	24.733	100.811	1.00	26.39
6118	C	ASN	B	19089	53.799	27.161	101.116	1.00	18.84
6119	O	ASN	B	19089	54.261	28.220	101.555	1.00	21.45
6120	N	PHE	B	1910	52.507	27.008	100.849	1.00	15.51
6122	CA	PHE	B	1910	51.591	28.107	101.082	1.00	13.39
6124	CB	PHE	B	1910	50.313	27.926	100.282	1.00	12.97
6127	CG	PHE	B	1910	49.208	28.833	100.724	1.00	11.32
6128	CD1	PHE	B	1910	48.234	28.374	101.569	1.00	12.24
6130	CE1	PHE	B	1910	47.208	29.226	102.002	1.00	13.55
6132	CZ	PHE	B	1910	47.199	30.528	101.583	1.00	14.09
6134	CE2	PHE	B	1910	48.155	31.001	100.765	1.00	15.47
6136	CD2	PHE	B	1910	49.182	30.170	100.333	1.00	15.53
6138	C	PHE	B	1910	51.209	28.174	102.548	1.00	12.51
6139	O	PHE	B	1910	50.906	27.158	103.153	1.00	11.67
6140	N	GLY	B	1921	51.198	29.373	103.116	1.00	11.05
6142	CA	GLY	B	1921	50.723	29.537	104.475	1.00	10.23
6145	C	GLY	B	1921	51.400	28.648	105.478	1.00	10.04
6146	O	GLY	B	1921	52.622	28.553	105.517	1.00	10.71
6147	N	GLU	B	1932	50.588	28.022	106.324	1.00	9.21
6149	CA	GLU	B	1932	51.080	27.161	107.376	1.00	9.64

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6151	CB	GLU	B	1932	50.161	27.254	108.603	1.00	9.93
6154	CG	GLU	B	1932	50.163	28.648	109.212	1.00	10.46
6157	CD	GLU	B	1932	49.321	28.814	110.460	1.00	13.61
6158	OE1	GLU	B	1932	48.270	28.150	110.584	1.00	13.90
6159	OE2	GLU	B	1932	49.687	29.663	111.305	1.00	13.61
6160	C	GLU	B	1932	51.185	25.756	106.827	1.00	9.07
6161	O	GLU	B	1932	50.346	24.883	107.066	1.00	8.71
6162	N	GLU	B	1943	52.206	25.558	106.017	1.00	9.53
6164	CA	GLU	B	1943	52.458	24.261	105.396	1.00	9.76
6166	CB	GLU	B	1943	53.031	23.286	106.397	1.00	10.77
6169	CG	GLU	B	1943	54.425	23.745	106.795	1.00	13.32
6172	CD	GLU	B	1943	54.995	22.943	107.934	1.00	16.94
6173	OE1	GLU	B	1943	55.872	22.095	107.676	1.00	20.88
6174	OE2	GLU	B	1943	54.556	23.160	109.083	1.00	20.48
6175	C	GLU	B	1943	51.240	23.722	104.677	1.00	9.20
6176	O	GLU	B	1943	50.919	22.535	104.744	1.00	10.36
6177	N	GLY	B	1954	50.587	24.614	103.954	1.00	8.73
6179	CA	GLY	B	1954	49.467	24.271	103.107	1.00	8.32
6182	C	GLY	B	1954	48.120	24.678	103.638	1.00	7.58
6183	O	GLY	B	1954	47.118	24.600	102.914	1.00	8.18
6184	N	TYR	B	1965	48.093	25.126	104.890	1.00	7.53
6186	CA	TYR	B	1965	46.878	25.464	105.599	1.00	8.13
6188	CB	TYR	B	1965	46.843	24.700	106.932	1.00	7.32
6191	CG	TYR	B	1965	46.661	23.229	106.695	1.00	7.26
6192	CD1	TYR	B	1965	47.734	22.424	106.339	1.00	5.84
6194	CE1	TYR	B	1965	47.565	21.078	106.107	1.00	6.72
6196	CZ	TYR	B	1965	46.298	20.546	106.163	1.00	6.85
6197	OH	TYR	B	1965	46.093	19.210	105.922	1.00	9.01
6199	CE2	TYR	B	1965	45.231	21.325	106.539	1.00	7.15
6201	CD2	TYR	B	1965	45.403	22.642	106.797	1.00	8.02
6203	C	TYR	B	1965	46.811	26.930	105.881	1.00	7.40
6204	O	TYR	B	1965	47.825	27.630	105.903	1.00	7.75
6205	N	ILE	B	1976	45.595	27.410	106.115	1.00	6.80
6207	CA	ILE	B	1976	45.395	28.791	106.499	1.00	6.47
6209	CB	ILE	B	1976	45.033	29.727	105.303	1.00	6.64
6211	CG1	ILE	B	1976	44.677	31.125	105.786	1.00	6.46
6214	CD1	ILE	B	1976	44.552	32.110	104.681	1.00	9.47
6218	CG2	ILE	B	1976	43.888	29.162	104.494	1.00	8.38
6222	C	ILE	B	1976	44.356	28.798	107.581	1.00	7.58
6223	O	ILE	B	1976	43.362	28.102	107.504	1.00	8.26
6224	N	ARG	B	1987	44.599	29.549	108.639	1.00	7.17
6226	CA	ARG	B	1987	43.602	29.693	109.687	1.00	7.14
6228	CB	ARG	B	1987	44.288	29.670	111.050	1.00	8.16
6231	CG	ARG	B	1987	44.727	28.302	111.416	1.00	9.63
6234	CD	ARG	B	1987	45.306	28.125	112.769	1.00	11.17
6237	NE	ARG	B	1987	46.603	28.731	112.890	1.00	13.37
6239	CZ	ARG	B	1987	47.314	28.674	113.998	1.00	18.33
6240	NH1	ARG	B	1987	46.871	27.970	115.042	1.00	22.48
6243	NH2	ARG	B	1987	48.514	29.260	114.043	1.00	17.78
6246	C	ARG	B	1987	42.881	31.006	109.402	1.00	8.08
6247	O	ARG	B	1987	43.505	32.042	109.276	1.00	9.33

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6248	N	MET	B	1998	41.582	30.936	109.175	1.00	7.33
6250	CA	MET	B	1998	40.792	32.082	108.759	1.00	7.98
6252	CB	MET	B	1998	40.034	31.726	107.487	1.00	8.23
6255	CG	MET	B	1998	40.942	31.351	106.346	1.00	10.02
6258	SD	MET	B	1998	40.132	31.141	104.757	1.00	11.68
6259	CE	MET	B	1998	39.516	32.850	104.490	1.00	11.24
6263	C	MET	B	1998	39.818	32.505	109.821	1.00	7.71
6264	O	MET	B	1998	39.229	31.676	110.508	1.00	8.46
6265	N	ALA	B	200199	39.632	33.806	109.955	1.00	7.99
6267	CA	ALA	B	200199	38.822	34.326	111.041	1.00	7.95
6269	CB	ALA	B	200199	38.722	35.831	110.954	1.00	8.38
6273	C	ALA	B	200199	37.438	33.726	111.098	1.00	8.08
6274	O	ALA	B	200199	36.748	33.645	110.092	1.00	8.33
6275	N	ARG	B	2010	37.043	33.311	112.297	1.00	7.98
6277	CA	ARG	B	2010	35.764	32.674	112.577	1.00	7.48
6279	CB	ARG	B	2010	35.990	31.306	113.221	1.00	8.59
6282	CG	ARG	B	2010	34.793	30.534	113.621	1.00	7.84
6285	CD	ARG	B	2010	35.111	29.079	113.972	1.00	8.20
6288	NE	ARG	B	2010	35.940	28.882	115.149	1.00	8.24
6290	CZ	ARG	B	2010	35.476	28.700	116.372	1.00	10.90
6291	NH1	ARG	B	2010	34.184	28.683	116.604	1.00	11.14
6294	NH2	ARG	B	2010	36.341	28.510	117.335	1.00	9.17
6297	C	ARG	B	2010	34.945	33.577	113.493	1.00	9.02
6298	O	ARG	B	2010	35.491	34.271	114.362	1.00	10.06
6299	N	ASN	B	2011	33.641	33.529	113.293	1.00	9.73
6301	CA	ASN	B	2021	32.703	34.336	114.066	1.00	10.02
6303	CB	ASN	B	2021	32.626	33.888	115.554	1.00	10.89
6306	CG	ASN	B	2021	32.101	32.453	115.704	1.00	14.32
6307	OD1	ASN	B	2021	31.303	32.014	114.895	1.00	18.88
6308	ND2	ASN	B	2021	32.539	31.729	116.726	1.00	16.87
6311	C	ASN	B	2021	32.979	35.817	113.899	1.00	10.95
6312	O	ASN	B	2021	32.809	36.594	114.843	1.00	12.12
6313	N	LYS	B	2032	33.398	36.204	112.692	1.00	10.42
6315	CA	LYS	B	2032	33.651	37.587	112.334	1.00	11.19
6317	CB	LYS	B	2032	35.135	37.834	112.084	1.00	12.43
6320	CG	LYS	B	2032	35.975	37.653	113.336	1.00	15.15
6323	CD	LYS	B	2032	35.945	38.858	114.265	1.00	18.00
6326	CE	LYS	B	2032	36.601	38.516	115.606	1.00	21.86
6329	NZ	LYS	B	2032	36.870	39.722	116.429	1.00	24.73
6333	C	LYS	B	2032	32.793	37.985	111.120	1.00	10.43
6334	O	LYS	B	2032	33.280	38.536	110.140	1.00	13.09
6335	N	GLY	B	2043	31.516	37.670	111.195	1.00	10.71
6337	CA	GLY	B	2043	30.568	38.087	110.179	1.00	9.73
6340	C	GLY	B	2043	30.758	37.394	108.856	1.00	9.79
6341	O	GLY	B	2043	30.698	38.048	107.805	1.00	10.48
6342	N	ASN	B	2054	30.947	36.084	108.895	1.00	8.78
6344	CA	ASN	B	2054	31.118	35.306	107.663	1.00	9.14
6346	CB	ASN	B	2054	29.816	35.287	106.847	1.00	8.57
6349	CG	ASN	B	2054	29.871	34.356	105.656	1.00	9.85
6350	OD1	ASN	B	2054	30.714	33.457	105.606	1.00	10.55
6351	ND2	ASN	B	2054	28.993	34.588	104.678	1.00	9.83

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6354	C	ASN	B	204 ——205	32.257	35.907	106.863	1.00	8.79
6355	O	ASN	B	2054	32.157	36.192	105.662	1.00	8.32
6356	N	HIS	B	2065	33.390	36.022	107.527	1.00	8.97
6358	CA	HIS	B	2065	34.562	36.629	106.946	1.00	9.36
6360	CB	HIS	B	2065	35.685	36.706	107.987	1.00	9.58
6363	CG	HIS	B	2065	36.709	37.718	107.620	1.00	12.39
6364	ND1	HIS	B	2065	37.991	37.377	107.263	1.00	16.98
6366	CE1	HIS	B	2065	38.649	38.469	106.928	1.00	11.60
6368	NE2	HIS	B	2065	37.842	39.504	107.058	1.00	16.78
6370	CD2	HIS	B	2065	36.609	39.059	107.462	1.00	13.69
6372	C	HIS	B	2065	35.015	35.885	105.718	1.00	9.31
6373	O	HIS	B	2065	35.164	34.675	105.738	1.00	9.77
6374	N	CYS	B	2066	35.224	36.627	104.637	1.00	9.31
6376	CA	CYS	B	2076	35.652	36.073	103.361	1.00	10.32
6378	CB	CYS	B	2076	37.034	35.443	103.460	1.00	10.86
6381	SG	CYS	B	2076	38.348	36.657	103.762	1.00	15.14
6382	C	CYS	B	2076	34.667	35.088	102.805	1.00	8.76
6383	O	CYS	B	2076	35.011	34.317	101.912	1.00	8.20
6384	N	GLY	B	2087	33.433	35.115	103.297	1.00	7.91
6386	CA	GLY	B	2087	32.406	34.217	102.775	1.00	7.40
6389	C	GLY	B	2087	32.603	32.747	103.107	1.00	7.54
6390	O	GLY	B	2087	32.037	31.862	102.490	1.00	8.17
6391	N	ILE	B	2098	33.398	32.476	104.126	1.00	8.18
6393	CA	ILE	B	2098	33.712	31.097	104.439	1.00	8.78
6395	CB	ILE	B	2098	34.717	31.038	105.588	1.00	9.19
6397	CG1	ILE	B	2098	35.228	29.592	105.723	1.00	11.64
6400	CD1	ILE	B	2098	36.618	29.494	106.171	1.00	12.80
6404	CG2	ILE	B	2098	34.102	31.548	106.878	1.00	10.66
6408	C	ILE	B	2098	32.479	30.221	104.693	1.00	8.02
6409	O	ILE	B	2098	32.464	29.036	104.334	1.00	7.30
6410	N	ALA	B	21009	31.429	30.780	105.285	1.00	7.38
6412	CA	ALA	B	21009	30.201	30.046	105.509	1.00	7.87
6414	CB	ALA	B	21009	29.674	30.319	106.921	1.00	8.78
6418	C	ALA	B	21009	29.136	30.362	104.478	1.00	7.92
6419	O	ALA	B	21009	27.971	30.007	104.685	1.00	9.05
6420	N	SER	B	2110	29.510	30.982	103.360	1.00	6.97
6422	CA	SER	B	2110	28.513	31.279	102.340	1.00	8.47
6424	CB	SER	B	2110	29.114	32.218	101.316	1.00	7.74
6427	OG	SER	B	2110	29.265	33.533	101.848	1.00	8.06
6429	C	SER	B	2110	27.970	30.016	101.677	1.00	8.53
6430	O	SER	B	2110	26.744	29.822	101.620	1.00	9.33
6431	N	PHE	B	2121	28.856	29.148	101.203	1.00	8.26
6433	CA	PHE	B	2121	28.425	27.984	100.461	1.00	8.97
6435	CB	PHE	B	2121	28.614	28.246	98.979	1.00	9.56
6438	CG	PHE	B	2121	27.776	29.395	98.473	1.00	11.11
6439	CD1	PHE	B	2121	28.340	30.628	98.234	1.00	11.91
6441	CE1	PHE	B	2121	27.553	31.693	97.786	1.00	13.66
6443	CZ	PHE	B	2121	26.200	31.515	97.613	1.00	15.69
6445	CE2	PHE	B	2121	25.622	30.283	97.876	1.00	15.67
6447	CD2	PHE	B	2121	26.412	29.234	98.312	1.00	13.06
6449	C	PHE	B	2121	29.162	26.729	100.890	1.00	8.20

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6450	O	PHE	B	2121	29.967	26.194	100.157	1.00	9.55
6451	N	PRO	B	2132	28.840	26.235	102.067	1.00	7.58
6452	CA	PRO	B	2132	29.467	25.028	102.573	1.00	7.51
6454	CB	PRO	B	2132	29.381	25.219	104.100	1.00	7.85
6457	CG	PRO	B	2132	28.799	26.602	104.314	1.00	8.37
6460	CD	PRO	B	2132	27.978	26.838	103.091	1.00	7.33
6463	C	PRO	B	2132	28.687	23.803	102.150	1.00	7.29
6464	O	PRO	B	2132	27.458	23.840	102.094	1.00	8.78
6465	N	SER	B	2143	29.388	22.716	101.906	1.00	7.32
6467	CA	SER	B	2143	28.730	21.454	101.622	1.00	8.06
6469	CB	SER	B	2143	28.403	21.347	100.149	1.00	8.21
6472	OG	SER	B	2143	29.575	21.438	99.349	1.00	9.81
6474	C	SER	B	2143	29.615	20.302	102.029	1.00	7.59
6475	O	SER	B	2143	30.833	20.443	102.149	1.00	7.85
6476	N	TYR	B	2154	29.003	19.152	102.241	1.00	8.34
6478	CA	TYR	B	2154	29.761	17.946	102.557	1.00	8.50
6480	CB	TYR	B	2154	30.026	17.772	104.056	1.00	8.96
6483	CG	TYR	B	2154	28.795	17.546	104.891	1.00	10.08
6484	CD1	TYR	B	2154	28.092	18.605	105.438	1.00	11.59
6486	CE1	TYR	B	2154	26.962	18.386	106.215	1.00	11.64
6488	CZ	TYR	B	2154	26.533	17.114	106.447	1.00	13.10
6489	OH	TYR	B	2154	25.386	16.889	107.201	1.00	16.38
6491	CE2	TYR	B	2154	27.208	16.054	105.925	1.00	12.70
6493	CD2	TYR	B	2154	28.337	16.268	105.155	1.00	11.46
6495	C	TYR	B	2154	29.038	16.745	101.993	1.00	8.54
6496	O	TYR	B	2154	27.802	16.728	101.924	1.00	9.15
6497	N	PRO	B	2165	29.798	15.762	101.557	1.00	8.44
6498	CA	PRO	B	2165	29.233	14.543	101.005	1.00	8.78
6500	CB	PRO	B	2165	30.322	14.095	100.028	1.00	8.88
6503	CG	PRO	B	2165	31.601	14.545	100.702	1.00	8.53
6506	CD	PRO	B	2165	31.277	15.741	101.519	1.00	8.41
6509	C	PRO	B	2165	29.083	13.482	102.059	1.00	10.39
6510	O	PRO	B	2165	29.679	13.557	103.117	1.00	10.24
6511	N	GLU	B	2176	28.299	12.469	101.743	1.00	10.96
6513	CA	GLU	B	2176	28.221	11.317	102.614	1.00	13.19
6515	CB	GLU	B	2176	27.005	11.396	103.549	1.00	15.26
6518	CG	GLU	B	2176	27.318	12.274	104.768	1.00	18.05
6521	CD	GLU	B	2176	26.124	12.591	105.663	1.00	22.53
6522	OE1	GLU	B	2176	26.097	12.144	106.848	1.00	27.25
6523	OE2	GLU	B	2176	25.227	13.303	105.189	1.00	22.86
6524	C	GLU	B	2176	28.321	10.075	101.731	1.00	13.81
6525	O	GLU	B	2176	28.107	10.120	100.521	1.00	13.33
6526	N	ILE	B	2187	28.704	8.968	102.344	1.00	14.68
6528	CA	ILE	B	2187	28.898	7.712	101.620	1.00	16.34
6530	CB	ILE	B	2187	30.356	7.277	101.777	1.00	16.17
6532	CG1	ILE	B	2187	31.211	8.231	100.959	1.00	17.81
6535	CD1	ILE	B	2187	32.681	8.041	101.087	1.00	19.32
6539	CG2	ILE	B	2187	30.577	5.862	101.271	1.00	17.38
6543	C	ILE	B	2187	27.899	6.654	102.079	1.00	18.67
6544	O	ILE	B	2187	27.164	6.116	101.235	1.00	21.88
6545	O5	E64	B	2198	34.121	30.173	90.104	1.00	26.67

FIGURE 3 (Cont.)

A	B	C	D	E	F	G	H	I	J
6546	C11	E64	B	2198	33.822	29.072	90.553	1.00	24.39
6547	C6	E64	B	2198	34.642	28.498	91.669	1.00	20.50
6549	C7	E64	B	2198	34.118	29.099	92.976	1.00	20.45
6552	C8	E64	B	2198	34.705	28.458	94.230	1.00	18.22
6554	C10	E64	B	2198	34.683	26.931	94.166	1.00	17.40
6558	C9	E64	B	2198	34.018	29.001	95.485	1.00	18.67
6562	N1	E64	B	2198	36.071	28.806	91.559	1.00	19.79
6564	C4	E64	B	2198	36.859	27.888	90.993	1.00	21.86
6565	O4	E64	B	2198	36.392	26.846	90.563	1.00	21.74
6566	C3	E64	B	2198	38.333	28.132	90.843	1.00	23.81
6568	O3	E64	B	2198	38.539	29.270	90.033	1.00	27.96
6570	C2	E64	B	2198	39.019	28.435	92.162	1.00	25.36
6573	C1	E64	B	2198	40.503	28.169	92.048	1.00	26.17
6574	O2	E64	B	2198	40.931	27.091	91.407	1.00	22.97
6576	O1	E64	B	2198	41.313	28.926	92.555	1.00	27.62
6577	N2	E64	B	2198	32.802	28.317	90.117	1.00	23.21
6579	C12	E64	B	2198	31.842	28.668	89.079	1.00	25.60
6582	C13	E64	B	2198	32.436	28.304	87.736	1.00	27.50
6585	C14	E64	B	2198	31.439	27.509	86.905	1.00	31.00
6588	C15	E64	B	2198	31.759	27.646	85.422	1.00	33.32
6591	N3	E64	B	2198	30.531	27.322	84.703	1.00	37.32
6593	C16	E64	B	2198	30.100	27.805	83.535	1.00	40.73
6594	N5	E64	B	2198	30.762	28.709	82.812	1.00	42.37
6597	N4	E64	B	2198	28.937	27.347	83.083	1.00	42.34
6600	O	HOH	W	1	65.010	24.930	63.116	1.00	55.52
6603	O	HOH	W	2	77.256	36.811	70.602	1.00	10.08
6606	O	HOH	W	3	47.993	24.927	100.087	1.00	8.83
6609	O	HOH	W	4	35.329	20.114	84.864	1.00	11.34
6612	O	HOH	W	5	33.947	15.288	105.007	1.00	9.78
6615	O	HOH	W	6	69.860	18.539	71.383	1.00	9.71
6618	O	HOH	W	7	51.786	20.083	103.934	1.00	12.76
6621	O	HOH	W	8	42.117	15.546	102.628	1.00	9.67
6624	O	HOH	W	9	34.089	34.712	110.116	1.00	9.09
6627	O	HOH	W	10	57.841	36.909	46.760	1.00	11.84
6630	O	HOH	W	11	84.176	34.864	53.493	1.00	11.13
6633	O	HOH	W	12	29.083	7.162	93.810	1.00	11.10
6636	O	HOH	W	13	63.992	42.975	56.093	1.00	10.67
6639	O	HOH	W	14	44.051	13.459	90.398	1.00	12.26
6642	O	HOH	W	15	47.954	17.469	105.221	1.00	9.60
6645	O	HOH	W	16	78.158	27.636	55.502	1.00	10.51
6648	O	HOH	W	17	29.801	9.397	105.035	1.00	12.95
6651	O	HOH	W	18	80.933	31.456	59.132	1.00	10.26
6654	O	HOH	W	19	66.723	29.785	75.948	1.00	11.37
6657	O	HOH	W	20	39.958	15.418	104.301	1.00	9.71
6660	O	HOH	W	21	31.652	29.091	101.619	1.00	8.26
6663	O	HOH	W	22	37.278	33.577	107.249	1.00	12.20
6666	O	HOH	W	23	68.372	36.610	82.094	1.00	11.82
6669	O	HOH	W	24	21.336	20.339	100.798	1.00	15.70
6672	O	HOH	W	25	80.910	33.978	60.177	1.00	10.81
6675	O	HOH	W	26	65.778	30.096	82.353	1.00	13.90
6678	O	HOH	W	27	40.211	8.325	102.491	1.00	11.50